14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Multi-Physics Modeling of Thermomechanical Response of Ultrasonically Activated Soft Tissue

Author(s): *Rahul , Suvranu De, *Rensselaer Polytechnic Inst.*.

Ultrasonic surgical instruments have been gaining popularity among surgeons in the last decade. An increasing number of surgical procedures including but not limited to head, neck, gynecological, colorectal and gastrointestinal surgeries are performed using ultrasonic surgical instruments [1]. These instruments utilize ultrasonic vibrations to cut, coagulate and dissect tissues, and seal vessels. They have been proven to be superior to conventional instruments and techniques such as electrosurgical and laser-based devices as they impose lesser thermal injury, desiccation and charring, lower mean blood loss during surgery, no risk of stray current, neuromuscular stimulation, lesser operation time and post-operative pain, and no smoke during the operation to occlude laparoscopic view [2]. Despite the increasing popularity of ultrasound-based surgical procedures, the affects of cellular level mechanisms on the thermomechanical response of ultrasonically activated soft tissues have not been understood completely. We have developed a multi-physics model to investigate the effects of cavitation, due to large transient pressure changes, on the thermomechanical response of soft tissue subjected to ultrasound vibrations [3]. Cellular level cavitation effects have been incorporated in the tissue level continuum model to accurately determine the thermodynamic states such as temperature and pressure. A viscoelastic material model is assumed for the macromechanical response of the tissue. The cavitation model based equation-of-state provides the additional pressure arising from evaporation of intracellular and cellular water by absorbing heat due to viscoelastic heating in the tissue, and temperature to the continuum level thermomechanical model. The thermomechanical response of soft tissue is studied for the operational range of frequencies of oscillations and applied loads for typical ultrasonically activated surgical instruments. The model is shown to capture characteristics of ultrasonically activated soft tissue deformation and temperature evolution. At the cellular level, evaporation of water below the boiling temperature under ambient conditions is indicative of protein denaturation around the temperature threshold for coagulation of tissues. Further, with increasing operating frequency (or loading), the temperature rises faster leading to rapid evaporation of tissue cavity water, which may lead to accelerated protein denaturation and coagulation. References: [1] Sankaranarayanan, G., Resapu, R.R., Jones, D.B., et al. (2013) Surg. Endosc. 27, 3056-3072. [2] Amaral, J. F., Chrostek, C. A. (1997) Minim. Invasive Ther. Allied Technol. 6, 324-331. [3] Rahul, De, S., (2017) Comput. Methods Appl. Mech. Eng. 314, 71-84.

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Title: Plastic Deformation and Non-linear Damage Evolution Modeling for Pipeline Steel

Author(s): *Hari Simha , *canmetMaterials, NRCAN*.

Field deformation data for X70 pipeline steel, obtained using digital-image correlation, is used to calibrate both plasticity and damage models. Experimental deformation fields were obtained on uni-axially loaded round bars, notched round bars, notched flat plates, and plates with a central hole. The well-known Hill48 model is used to describe yield and anisotropy of strength. Using virtual extensometers that are strategically located, anisotropy coefficients are calibrated using the DIC data. Implicit finite element simulations using the Abaqus finite element software are used for the latter effort. Onset of localization and subsequent damage evolution is modeled using the frameworks developed by Wierzbicki and co-workers, [1, 2]. A strain-based failure surface that depends on both the Lode angle (third invariant of the stress tensor) and the tri-axiality (second invariant of the stress tensor) is used as the threshold for localization. The novelty in the damage model is the use of an evolution law that is reminiscent of the flow curves used in unified plasticity; specifically, the Bodner-Partom model, [3]. On account of this model, low values of damage exists at all load levels, but starts to grow significantly only when the localization threshold described by the failure surface is exceeded. This feature circumvents the need to assume damage levels greater than unity to model crack propagation. The damage-mechanics framework is implemented in Abaqus/explicit. To mitigate mesh dependence owing to softening of the strength, a non-local approach is used. Examples of ductile damage propagation in compact and single edged notch tension samples are shown. Particularly, the importance of the Lode angle in modeling the flat-to-slant transition in crack propagation is emphasized. Where possible, fracture mechanics experiments are modeled using the developed framework. [1] Bai, Y. and Wierzbicki, T., 2008. A new model of metal plasticity and fracture with pressure and Lode dependence. International journal of plasticity, 24(6), pp.1071-1096. [2] Xue, L. and Wierzbicki, T., 2008. Ductile fracture initiation and propagation modeling using damage plasticity theory. Engineering Fracture Mechanics, 75(11), pp.3276-3293. [3] Bodner, S. and Partom, Y., 1975. Constitutive equations for elastic-viscoplastic strain-hardening materials. Journal of Applied Mechanics, 42(2), pp.385-389.

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Title: An Equation-Free Multiscale Method: Extension of the Quasicontinuum Method to Irregular Structures

Author(s): *Lars A.A. Beex, *University of Luxembourg*; Pierre Kerfriden, *Cardiff University*.

The quasicontinuum (QC) method was first developed to reduce computational costs of atomistic computations [1]. It allows one to preserve the full atomistic description in small regions of interest and to coarse-grain the atomistic model elsewhere. As such, it combines aspects of reduced order modelling approaches and concurrent multiscale approaches. For two decades, the QC method was only applied to conservative atomistic models. Not long ago however, it was extended towards discrete dissipative models that can for instance be used to model fibre networks, foams and printed structures [2]. The extension to beam models also enlarged its application range [3]. An important drawback of the QC method is that it can only be applied to lattice models (in which each node/atom is connected to its neighbouring nodes/atoms in the same manner). Work was performed to extend the method towards irregular discrete models and resulted in QC approaches that show similarities to FE2 approaches. Consequently, those extensions come with similar advantages and disadvantages as computational homogenisation approaches. In this presentation we will show a different extension of the QC method towards irregular discrete models. The extension is e ffectively a numerical generalisation of the QC method and has the advantage that the resulting framework remains fully nonlocal. Consequently, the approach can relatively straightforwardly be employed for higher-order interpolation schemes at the macroscale. This will be demonstrated by higher-order examples in which irregular, planar beam models with damage are considered. We consider that the resulting approach has two main advantages. First, no macro-to-micro and micro-to-macro relations need to be de fined. This means amongst others that no boundary conditions at the microstructure need to be applied. This is an advantage because for higher-order interpolation fi elds at the macroscale, these boundary conditions are not trivial. The second advantage is that the separation-of-scales principle does not apply to the method. Hence, the user does not have to worry if scale separation is present. References [1] E.B. Tadmor, R. Phillips, M. Ortiz, "Mixed atomistics and continuum models of deformation in solids", Langmuir, v. 12, p. 4529-4534, 1996. [2] L.A.A. Beex, R.H.J. Peerlings, M.G.D. Geers, "A multiscale quasicontinuum method for dissipative lattice models and discrete networks", Journal of the Mechanics and Physics of Solids, v. 64, p. 154-169, 2014. [3] L.A.A. Beex, P. Kerfriden, T. Rabczuk, S.P.A. Bordas, "Quasicontinuum-based multiscale approaches for plate-like beam lattices experiencing in-plane and out-of-plane deformation", Computer Methods in Applied Mechanics and Engineering, v. 279, p. 348-378, 2014.

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Title: Experimental Observation of Multiscale Deformation in Heterogeneous Materials Subjected to Impact Loading

Author(s): * Addis Kidane Suraj Ravindran , *kidanea@cec.sc.edu*.

The deformation of heterogeneous materials is multi-scale and need a multi-scale approach to fully understand the underline failure mechanisms. When subjected to dynamic loadings such as impact and blast loading, the failure mechanism in heterogeneous materials becomes more complex. Bridging the failure mechanisms that are observed at different length scales has been a great interest in both computational and experimental mechanics community. With the objective of understanding the failure mechanisms of heterogeneous materials subjected to impact loading, full field image based experiments, at two different scales, are conducted. The material used for the study is polymer bonded sugar, a heterogeneous material where a solid sugar crystal is bonded with a polymer matrix. The experiments are conducted using Hopkinson pressure bar apparatus in direct impact configuration, where the projectile is directly shot at the specimen. Series of experiments are conducted at different impact velocities. At macroscale level using the full field strain obtained from digital image correlation, the compaction wave thickness and velocity are calculated. Furthermore, using displacement field and non-parametric methods, the compaction stress across the specimen is calculated. The energy absorbed in the material is also calculated. At mesoscale, the local deformation, such strain in each grain and around the boundary is measured. The information obtained at mesoscale is used to explain the energy dissipation mechanism observed at the macroscale.

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Title: A Dynamic Variational Multiscale Method for Viscoelasticity Using Linear Tetrahedral Elements

Author(s): *Nabil Abboud, Oriol Colomes, Guglielmo Scovazzi, *Duke University*.

We propose an extension of the dynamic variational multiscale stabilization (D-VMS) to nearly/fully incompressible viscoelastic materials using quadrilateral/tetrahedral finite elements. The viscous behavior of the material is modeled using prony series expansions which are common in the practice of finite element simulations. Our method is based on a mixed formulation, in which the momentum equation is complemented by a pressure equation in rate form. The unknown pressure, displacement and velocity are approximated with piecewise linear, continuous finite element functions. In order to prevent spurious oscillations, the pressure equation is augmented with a stabilization operator specifically designed for viscoelastic problems, in that it depends on the viscoelastic dissipation.

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Title: Stochastic Uncertainties Analysis in Dam Break Flow Modeling Using a Reduced Order Model

Author(s): *Azzedine Abdedou, Azzeddine Soulaïmani, *École de Technologie Supérieure*; Jean-Marie Zokagoa, *University of Felix H. Boigny, Abidjan, Ivory Coast*.

The interest in dam break flow modeling has been increased considerably these last two decades due to the multiplication of extreme meteorological events. Thus, various numerical models have been developed to reproduce the real physical aspect of these phenomena and to forecast the arising consequences. Nonetheless, the physical parameters, initial and boundary conditions, on which these models are based, are often considered uncertain. The main objective of this work is to carry out a stochastic analysis of uncertainties propagation through the numerical free surface flow model by using Monte Carlo-type and Polynomial Chaos Expansion methods. The uncertain input data such as the inflow discharge, upstream water free surface elevation and Manning roughness coefficient are modeled as random variables which are generated according to their prescribed probability density function (PDF). For each set of random input parameters values, the simulations are then conducted using a deterministic in-house finite volume solver of the shallow water equation called CUTEFLOW. Uncertainties analysis becomes thus prohibitive due to the large number of executions required to achieve an acceptable accuracy. Therefore, we consider also the use of the corresponding reduced order model which is based on the proper orthogonal decomposition method (Zokagoa and Soulaïmani, 2011 and 2012). Preliminary numerical tests have been conducted, and the results will be assessed through statistical estimators. Comparisons between the full and reduced order models will give insight on the performance of the reduction methodology. A sensitivity analysis will also be performed in order to evaluate the contribution degree of each input parameter on the uncertainties of the output such as the position of the water-land frontier. References Zokagoa, J.-M. and Soulaïmani A. 2011. A POD-based reduced-order model for free surface shallow water flows over real bathymetries for Monte-Carlo-type applications. Computer Methods in Applied Mechanics and Engineering. 221-222: 1-23. Zokagoa, J.-M. and Soulaïmani A. 2012. Low-order modelling of shallow water equations for sensitivity analysis using proper orthogonal decomposition. International Journal of Computational Fluid Dynamics 26 (5): 275-295. Ruiz-Bellet, J. L., Castelltort X., Carles Balasch J. and Tuset J. 2017. Uncertainty of the peak flow reconstruction of the 1907 flood in the Ebro River in Xerta (NE Iberian Peninsula). Journal of Hydrology 545 : 339–354.

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Title: Deformation of Polycrystals at Multiple Scales: Linking 3D-XRD to CPFE Modelling

Author(s): *Hamidreza Abdolvand, *Western University* ; Jonathan Wright, *ESRF*; Angus Wilkinson, *University of Oxford*.

There is a growing need to develop material constitutive equations that can accurately model deformation of polycrystalline materials at multiple length scales. Such need cannot be addressed unless reliable experimental data are provided to validate the assumptions made in the model. One of the experimental techniques that has played a key role in fulfilling such task is synchrotron x-ray diffraction. In this study, crystal plasticity finite element (CPFE) technique is linked to three-dimensional synchrotron x-ray diffraction technique (3D-XRD) to study deformation of individual grains of a commercially pure zirconium sample. While macroscopic deformation of the polycrystal is studied, it is tried to determine which slip systems are active at the room temperature. With the use of 3D-XRD, the centre of mass, relative volume, crystallographic orientation, and stress of more than 11000 grains were measured at various steps during a uniaxial loading. The 3D measured microstructure was subsequently imported into a CPFE code for simulating deformation of individual grains. Activity of each slip mode is studied and through examining their influence on the diffraction peak broadening, it is concluded that for the studied case, only basal and prism are the dominant slip mechanisms.

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Title: Development of Origin-Destination Matrix Estimation Method for Microscopic Traffic Simulator as Quadratic Programming

Author(s): *Kazuki Abe, Hideki Fujii, Shinobu Yoshimura, *The University of Tokyo*.

Nowadays, multi-agent-based microscopic traffic simulators are useful for making decisions for traffic-related problems, e.g. traffic jams, evacuation planning, etc. Traffic demand is one of the necessary input data for such simulators, which is described in the form of Origin-Destination (OD) matrix. Since the matrix cannot be observed directly, some indirect estimation methods are proposed so far. One of them uses link traffic volume, which can be observed at a fixed-point on the road. We propose a new method of the link-traffic-volume-based OD matrix estimation using a traffic simulator, which estimates the input data for the simulator itself. The proposed OD estimation method mainly consists of the following two processes: (1) a process of calculating estimated link traffic volume from the assumed OD matrix, and (2) a process of updating OD matrix with some constraints. In process (1), a microscopic traffic simulator ADVENTURE_Mates[1, 2] developed by the authors is used. In process (2), a new OD matrix is obtained by solving a quadratic programming (QP) problem. In this process, the residual, between the estimated link traffic volume and observed one, will be minimized with the constraint of non-negative traffic volume. In the formulation of the QP, we employ an assignment matrix, by which estimated link traffic volume is calculated from the assumed OD matrix. The assignment matrix is approximated from the result of the simulation in process (1), and it is valid around the current assumed OD matrix. For this reason, these processes should be iterated: until the norm of the residual satisfies a convergence criterion, the OD matrix should be updated repeatedly. When a stochastic simulator is used in the process (1), the timing that vehicles emerge, disappear or go through the observation point can change and consequently the result can be scattered. It causes that the precision of the approximated assignment matrix gets worse. Now, we find some valid approximation method for the assignment matrix and verify them by applying the method to some cases in the real world. References: [1] S. Yoshimura, MATES: Multi-Agent Based Traffic and Environment Simulator -- Theory, Implementation and Practical Application, Computer Modeling in Engineering and Sciences, Vol. 11, No. 1, 2006, pp. 17-25. [2] H. Fujii, S. Yoshimura, K. Seki, Multi-agent Based Traffic Simulation at Merging Section Using Coordinative Behavior Model, Computer Modeling in Engineering and Sciences, Vol. 63, No. 3, 2010, pp. 265-282.

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Title: Effect of Loading Rate and In-Situ Stress Anisotropy on Fracture Patterns in a Tight Formation

Author(s): *Reza Abedi, *University of Tennessee Space* ; Omid Omidi, *University of Kansas*; Philip Clarke, *University of Tennessee Space Institute*; Robert Haber, *University of Illinois at Urbana-Champaign*.

Hydraulic fracturing has been the most common approach to stimulate tight formations. The geometry of the wellbore and the time history of the hydraulic loading play important roles in induced fracture patterns. For example, generating multiple perforations in a wellbore to enhance its hydrocarbon recovery is nowadays attracting more attention. The increased number of fractures can potentially enhance the yield of a reservoir by increasing the regions affected by hydraulic fractures. However, in practice many of the initial perforations do not result in any substantial hydraulic crack propagation. Dynamic stimulation methods are often associated with explosive or propellant methods. These approaches are typically performed without any initial perforations. However, recent studies show that by using a hybrid approach, in which similar to hydraulic fracturing there are some initial perforations but for these high loading rate conditions, all perforations can be activated, thus affecting larger areas of the reservoir. We study the conditions for which the initial perforations become effective and propagate in rock. We combine the asynchronous spacetime discontinuous Galerkin method with an interfacial damage model in our fracture simulations. Mesh adaptive schemes are used to align crack trajectories with inter-element boundaries. We consider loading rates ranging from 10 microseconds to 1 second. The first few high loading rates are hypothetical and are included to better demonstrate the effect of fracture strength randomness on fracture response. The loading rates from 1 to 100 milliseconds correspond to the aforementioned hybrid methods, while lower rates can be associated with very early stages of hydraulic fracturing. Our numerical results show that at low loading rates only a few of the initial perforations become active. As the loading rate increases, more perforations become active until ultimately all result in crack propagation. Moreover, higher loading rates affect larger zones for each of the initial perforations by dynamic fracture features such as microcracking and crack bifurcation. In-situ stress anisotropy has an adverse effect in that it prohibits activation of more perforations even at higher loading rates. Finally, we study the effect of spatial inhomogeneity of fracture strength on generated fracture patterns; as the loading rate increases a deterministic model, which assumes fracture strength is spatially uniform, starts to induce more microcracking and crack branching events. Accordingly, these studies imply the high impact of local material inhomogeneities on fracture response, particularly at high loading rates.

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Title: Developing Mesoscale Probabilistic Characterizations of the Elastic and Inelastic Properties of Random Composites Using Statistical Volume Elements

Author(s): *Katherine Acton, Sarah Baxter, *U. St Thomas*; Bahador Bahmani, Reza Abedi, *U. Tennessee Space Inst.*.

Representative volume elements (RVE) are often used as the basis for defining the effective properties of a composite material. While this is a powerful approach for predicting global response, it does not capture the inherent local variability. A meso-scale analysis based on partitions of an RVE, known as statistical volume elements (SVEs) can capture local variability by characterizing a distribution of properties approximating that present in the RVE sample. Previous work, on elastic properties, has demonstrated that how an RVE is partitioned is critical to a consistent analysis. Voronoi tessellation, in particular, has been shown able to capture subtle microstructural differences, is less sensitive to contrast ration between the phases, and provides more consistent distributions across a range of partition sizes.. In this work, the Voronoi tessellation based SVE analysis is extended to consider inelastic effects.

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Title: From Mesoscopic to Macroscopic Computations of Dynamic Contact Lines

Author(s): *Shahriar Afkhami, *NJIT*.

Contact lines that form when fluid-fluid interfaces intersect with solid boundaries are ubiquitous in industrial and natural applications, such as micro-nanofluidics and immiscible flows in porous media. Significant progress has been made recently on the modeling of dynamic contact line problems, yet they remain computationally difficult to tackle in that they involve length scales ranging from molecular to macroscopic scales. Here we present a review of the moving contact line paradox and present two approaches to eliminate it. The first approach is based on the inclusion of fluid-solid intermolecular interactions into the Navier-Stokes equations, and the second approach is based on a Volume-of-Fluid model where the boundary conditions are modified by introducing a slip model. In both models, we suggest a manner in which simulations can be carried out, despite the singularity at the contact line.

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Title: Parameter Estimation and Design of Experiments for Soft Tissues

Author(s): *Ankush Aggarwal, *Swansea University*.

Motivated by the well-known result that stiffness of soft tissue is proportional to the stress, many of the constitutive laws for soft tissues contain an exponential function. In this work, we analyze properties of the exponential function and how it affects the estimation and comparison of elastic parameters for soft tissues. In particular, we find that as a consequence of the exponential function there are lines of high covariance in the elastic parameter space. As a result, the functional contains a long narrow valley in the parameter space, which results in an ill-conditioned system and extremely slow convergence during the parameter estimation. We divide the parameter estimation problems into two categories: displacement-controlled (DC) and force-controlled (FC) cases. We use ideas from elementary algebra and extend those ideas to propose simple changes in the norm and the parameter space, which significantly improve the convergence of parameter estimation and robustness in the presence of noise. More importantly, we demonstrate that these changes improve the conditioning of the problem and provide a more robust solution in the case of heterogeneous material by reducing the chances of getting trapped in a local minima. We also found that FC problems might be better suited for parameter estimation. Furthermore, while performing the parameter estimation two important considerations arise: first, what is the effect of measurement errors/noise; and second, given the measurement errors what are the optimal locations (both in space and time) for taking the measurements. We provide preliminary results on these two considerations.

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Title: Analytical and Computational Investigation of Properties of a Linealy Elastic Peridynamic Material

Author(s): *Adair Aguiar, Alan Seitenfuss, *University of São Paulo*.

This work concerns a study of the properties of a linear elastic peridynamic material in the context of a three-dimensional state-based peridynamic theory, which considers both length and relative angle changes, and is based upon a free energy function that contains four material constants. Using convergence results of the peridynamic theory to the classical linear elasticity theory in the limit of vanishing sequences of the horizon and a correspondence argument between the proposed free energy function and the strain energy density function from the classical theory, expressions were obtained by Aguiar e Fosdick [2014] and Aguiar [2016a, 2016b] relating three peridynamic constants to the classical elasticity constants of an isotropic linearly elastic material. To evaluate the fourth peridynamic material constant, the correspondence argument is used together with the deformation field of an elastic beam subjected to pure bending. Other experiments in mechanics are then used to verify these evaluations. References [2014] A.R. Aguiar and R. Fosdick. A constitutive model for a linearly elastic peridynamic body. Mathematics and Mechanics of Solids, 19(5):502-523. [2016a] A.R. Aguiar. On the determination of a peridynamic constant in a linear constitutive model. Journal of Elasticity, 122:27-39. [2016b] A.R. Aguiar. Erratum to: On the determination of a peridynamic constant in a linear constitutive model. Journal of Elasticity, 122:41-42. Acknowledgements The authors acknowledge the support of CNPq, under grant 444896/2014-7.

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Title: Uncertainty Aware Topology Optimization via a Stochastic Reduced Order Model Approach

Author(s): *Miguel Aguilo, *Sandia National Laboratories* ; James Warner, *NASA Langley Research Center* .

This work presents a stochastic reduced order modeling strategy for the quantification and propagation of uncertainties in topology optimization. Uncertainty aware optimization problems can be computationally complex due to the substantial number of model evaluations that are necessary to accurately quantify and propagate uncertainties. This computational complexity is greatly magnified if a high-fidelity, physics-based numerical model is used for the topology optimization calculations. Therefore, we propose to apply stochastic reduced order model (SROM) methods to effectively 1) alleviate the prohibitive computational cost associated with an uncertainty aware topology optimization problem; and 2) quantify and propagate the inherent uncertainties due to design imperfections. We will present a generic SROM framework that transforms the uncertainty aware, stochastic topology optimization problem into a deterministic optimization problem that relies only on independent calls to a deterministic numerical model. This approach facilitates the use of existing optimization and modeling tools to accurately solve the uncertainty aware topology optimization problems in a fraction of the computational demand required by Monte Carlo methods. Finally, several examples in compliance and stress minimization are presented to demonstrate the robustness and effectiveness of the proposed uncertainty aware topology optimization approach.

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Title: Efficient Interlayer Modeling and Dynamic Fracture Analysis for Multilayered Structures with Peridynamics

Author(s): Youn Doh Ha, *Tae Sik Ahn, *Kunsan National University*.

An efficient interlayer modeling described by fictitious bonds is proposed in bond-based peridynamics. Utilizing it, multilayered structures in which every layer combines to each other with an interlayer material can be modeled and analyzed efficiently. In the previous study [1], a seven-layered glass structure with a polycarbonate backing was modeled by peridynamics and various dynamic fracture characteristics, such as Hertz-type cracks, compact region, ripple cracks, florets, etc., under a high-velocity impact on the top layer was investigated. However, there was no interlayer binding which exists in experiments and the penetration between layers was prevented by short-range interaction forces. In a typical peridynamic modeling, huge particles are required for a multilayered structure with very thin interlayers. Instead, in this study a few fictitious particles are distributed in the interlayer region. The interlayer bonds of those fictitious particles are implemented in peridynamic equations and bind neighboring layers. The efficiency of the developed interlayer modeling is verified through numerical examples. Also, fracture patterns for multilayered structures with interlayer bonding are compared with those excluding interlayer bonding. References: [1] Bobaru, F., Ha, Y. D., Hu, W., Damage Progression from Impact in Layered Glass Modeled with Peridynamics, Cent. Eur. J. Eng., 2(4), 2012, pp. 551~561.

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Title: Engineered Architected Materials: Multidirectional Functionally Graded Cellular Solids

Author(s): Hamed Niknam Jahromi, *Hamid Akbarzadeh, Armin Mirabolghasemi, *McGill University*; Denis Rodrigue, *Université Laval*; Daniel Therriault, *Ecole Polytechnique Montreal*.

Inspired by natural materials like bamboo and tooth enamel, the concept of multidirectional functionally graded cellular materials (MFGCM) is introduced in this investigation. MFGCMs consist of two engineered spatially-varying phases: solid and void. These engineered architected materials can be made by assembling unit cells of alternative cell relative densities, cell topologies, and cell orientations. These parameters can be tailored in multiple directions within the functionally graded cellular media in order to optimize their multiphysical properties. To evaluate the potential of MFGCMs to reduce structural weight and increase the multifunctional performance of structural elements, an attempt has been made to first analyze the mechanical and thermal properties of MFGCM structures and then manufacture these engineered architected materials through 3D printing. As two case studies, the thermomechanical properties of a novel moderately-thick MFGCM plate are improved by tailoring the microarchitecture of constitutive unit cells of periodic porous materials. A standard mechanics homogenization technique is implemented to predict the mechanical and thermal properties of cells of arbitrary two- and three-dimensional architecture. The homogenized effective properties along with finite element method and a higher-order shear deformation plate theory are exploited to predict the mechanical and thermal responses of MFGCMs, a new category of advanced materials which can be fabricated with additive manufacturing techniques. The aim is to establish benchmark results for exploring the potential of graded porous materials for achieving the optimized multifunctional properties through tuning the relative density, cell topology, and cell orientation within the MFGCMs. Finally, MFGCM structures with optimized mechanical and/or thermal properties are 3D printed to confirm their manufacturability for wider range of engineering applications.

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Title: Adaptivity of a B-Spline Based Finite-Element Method for Modelling Wind-Driven Ocean Circulation

Author(s): *Ibrahim Al balushi, Gantumur Tsogtgerel, *McGill University*; Wen Jiang, *Idaho National Laboratory*; Tae-yeon Kim, *Khalifa University*.

We present an adaptive refinement algorithm of a B-spline based finite-element approximation of the streamfunction formulation for the large scale wind-driven ocean currents. In particular, we focus on a posteriori error analysis of the simplified linear model of the stationary quasi-geostrophic equations, namely the Stommel-Munk model, which is a fourth-order partial differential equation. The analysis provides an a posteriori error estimator for the local refinement of the Nitsche-type finite-element formulation using cubic B-splines. Numerical experiments with several benchmark examples are performed to test the capability of the posteriori error indicator on rectangular and L-shape geometries.

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Title: Computational Framework for Homogenization at Finite Deformation with Stability Considerations Using Isogeometric Analysis

Author(s): *Ryan Alberdi, Kapil Khandelwal, *University of Notre Dame*.

A numerical framework for performing computational strain-driven, stress-driven and mixed homogenization at finite deformations is presented. A nested Newton-Raphson solution strategy is proposed to handle the issue of implementing stress-driven and mixed computational homogenization in a consistent manner. In addition, instabilities that may occur during finite deformations are taken into consideration. Bifurcation analysis performed at the microscale allows for the identification of modes that result in a loss of material stability at the macroscale. The proposed homogenization framework is developed for use with standard finite element analysis (FEA) as well as isogeometric analysis (IGA). Results using strain-driven, stress-driven and mixed homogenization with IGA are compared to those using FEA in order to assess the advantages of the approach. Additionally, examples utilizing detailed microscopic geometries that are difficult to mesh with FEA are presented and analyzed using IGA. These examples highlight how the isogeometric framework allows for efficient homogenization and stability analysis of intricate microstructural designs. Linking these designed microstructures to their macroscopic properties and determining ranges of stable macroscopic behavior has implications for the design of metamaterials with enhanced mechanical properties. Keywords: Multiscale stability; Finite deformation; Stress/strain driven homogenization; Isogeometric analysis; Metamaterials.

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Title: Energy Release Rate Approximation for Surface Cracks Using Topological Derivatives

Author(s): *Kazem Alidoost, Meng Feng, Philippe H. Geubelle, Daniel A. Tortorelli, *University of Illinois*.

Topological derivatives provide the variation of a functional when an infinitesimal hole is introduced into the domain. In a previous study, the authors developed a first-order approximation of the energy release rate associated with a small surface crack at any boundary location and at any orientation using a first-order topological derivative [1]. This approach offers significant computational advantages over other methods because (i) it requires only a single analysis while other methods require an analysis for each combination of location and orientation, and (ii) it is performed on the non-cracked domain, removing the need to create very fine meshes in the vicinity of crack tips. This initial study, however, was limited to small cracks in 2-D domains. In this work, a higher-order approximation of the energy release rate is developed using higher-order topological derivatives. In addition to the stress state present at the crack initiation point, this higher-order approximation incorporates the derivatives of the stress state computed on the uncracked domain in the expected direction of crack propagation. The derivatives of the stress state are computed using an asymptotic expansion for the tractions along the crack surface as the crack length approaches zero. Higher-order approximations allow the analyst to accurately treat longer cracks and determine for which crack lengths the first-order approximation is accurate. In this presentation, we begin by reviewing the first-order approximation of the energy release rate. We then combine this first-order approximation with Abaqus FEA so that simply by supplying an ODB file the first-order approximation of the energy release rate is computed for a crack at any boundary location and at any orientation. In this way, we promptly identify the critical combinations of boundary locations and orientations that reach the critical energy release rate at the smallest crack lengths. Subsequently, we introduce the higher-order approximations of the energy release rate and the asymptotic expansion used to calculate them. We conclude by showing how these higher-order approximations (i) increase the accuracy of the approximation when treating long cracks, and (ii) are used to predict for what crack sizes the first-order approximation is accurate. References: [1] M. Silva, P.H. Geubelle, D.A. Tortorelli, Energy release rate approximation for small surface-breaking cracks using the topological derivative, J. Mech. Phys . Solids, 59 (5) (2011), pp. 925–939.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Low Order Modeling for Structural Response of Columns under Extreme Loadings

Author(s): *Navid Allahverdi, *New York City College of Tech*; Ala Saadeghvaziri, *New Jersey Institute of Tech*.

This presentation discusses a methodology to build simplified low order models to predict structural response of stand-alone columns under extreme loadings. Low order models are built and characterized based on detailed high fidelity simulations. The underlying high fidelity simulation takes into account the coupled response of a column subjected to an incident overpressure propagating in a compressible fluid to represent air medium. The compressible fluid response is governed by Euler's equations in conjunction with Ideal gas equation-of-state. The air domain is discretized with Eulerian grids while columns are modeled with Lagrangian hexahedral elements. The proposed low order model for the column response consists of a single-degree of freedom (SDOF) model. The parameters of the equivalent single-degree of freedom are calibrated to match the response obtained from high fidelity simulation results. Forces imparted to the SDOF model are evaluated as a function of the shape and size of columns as well as the intensity of the blasts. Columns' shape and size influence the flow field in the vicinity of the column and forces experienced by the column as such. Based on the high fidelity simulations, force and impulse experienced by columns with different cross sectional shapes and varying sizes are estimated; and proper equations are proposed to estimate the force on columns based on shape, and size for a range of blast intensities using regression analysis. The blast intensity is represented via scaled distance. The proposed force/impulse equations in conjunction with the low order model (SDOF) provide a computationally cheap yet accurate estimation of the column response under extreme loadings and eliminate the need to perform computationally expensive high fidelity simulations.

14th U.S. National Congress on Computational Mechanics
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Title: Modeling the Effects of Microstructure on Localization in Polycrystalline Stainless Steel

Author(s): *Coleman Alleman, James Foulk, Alejandro Mota, Hojun Lim, David Littlewood, *Sandia National Laboratories*.

In a polycrystalline aggregate, the heterogeneous plastic deformation introduced by the local anisotropy of the microstructure plays a critical role in the localization of the deformation. To accurately resolve this incipient stage of failure, it is therefore necessary to incorporate microstructure with sufficient resolution, including accurate representations of interfaces such as grain boundaries. However, modeling the entire body at the required level of resolution is computationally prohibitive. In this study, the authors demonstrate the use of concurrent multiscale modeling to incorporate explicit, finely resolved microstructure in a critical region while resolving the smoother mechanical fields outside this region with a coarser discretization to limit computational cost. The Schwarz alternating method is a well-established technique for the solution of elliptic PDEs by means of domain decomposition. This concurrent multiscale method enables the flow of information between fine and coarse scales to achieve strong two-way coupling, which is critical in the accurate simulation of localization of plastic deformation leading to void or crack initiation in the incipient failure regime. The Schwarz method avoids the use of Lagrange multipliers or gradients that afflict other coupling methods, instead directly imposing the solution of each domain on the others in a way that guarantees convergence of the combined problem. This presentation will discuss the formulation of the Schwarz method and its implementation in the open-source Albany finite element platform developed at Sandia National Laboratories and demonstrate the use of the method as an effective approach for concurrent coupling in finite deformation solid mechanics. In particular, the Schwarz method is applied in this study to analyze the behavior of stainless steel tension specimens undergoing the localization of plastic deformation during the necking process. The gauge section of the specimen--where localization occurs--is resolved at a scale where the polycrystalline microstructure is discretized explicitly, and an anisotropic crystal elasto-viscoplasticity constitutive model is employed. The far field domain is coarsely discretized, and a simplified, isotropic elastoplastic constitutive relation is employed to capture the aggregate response of a polycrystalline region in a phenomenological manner. A suite of microstructural realizations are simulated to investigate the effects of microstructural variability on the necking process. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: Non-Intrusive Local-Global Substitution Method: Extension to Multi-Time and Jump Cycle Coupling for the Fatigue Prediction of Viscoplastic-Structures

Author(s): *Olivier Allix, Maxime Blanchard, Pierre Gosselet, *LMT-Cachan, ENS-Paris-Saclay.*; Geoffrey Desmeure, *Safran Aircraft Engines*.

This paper discusses new developments of a non-intrusive substitution approach for local-global computation in case of visco-plastic structures and low-cycle simulations. The “substitution” method proposed in previous works allows taking advantage of economical global coarse meshes, typically used in an industrial applications, and running separate local analyses only where needed in critical areas where structural details require refined meshes. A first issue, which is addressed in the presentation, deals with consistent integration at the local and global level in case of automatic sub-stepping (also cutbacks) as performed in Abaqus for example. Different strategies will be presented and compared on basic 2D examples and 3D ones. A second issue concerns the extension of the strategy in case of jump-cycles approaches in order to be able to analysis the visco-plastic response of complex structures over hundred of cycles and to predict the limit cycle.

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Title: Modeling of the Effects of Microstructure Variations in Li-ion Intercalation Batteries during Impact

Author(s): *Srikanth Allu, Srdjan Simunovic, Sergiy Kalnaus, Hsin Wang, John Turner, *Oak Ridge National Laboratory*.

Impact safety is an important design aspect of lithium-Ion batteries because an internal short can lead to the thermal runaway. We have developed a 3D multi-physics model of species transport, charge conservation and chemical kinetics for lithium-Ion batteries that uses a rigorous volume averaging approach based on a single formulation across the electrode-electrolyte-electrode system. In this approach, we can model the spatio-temporal gradients at the cell level informed by the closure relations from lower length scale. The performance model of the Li-Ion pouch cell has been validated against the experimental data at various discharge rates [1]. But to accurately predict the internal short we need to capture the deformed material variations. We will present analysis on microstructure reorganization during mechanical impact and the influence that it has on upscaled effective properties for electrochemical transport. The coupled electrochemical-thermal simulations based on the upscaled properties help us understand the underlying physical mechanisms that battery undergoes during the onset of internal short during crash. Reference: 1. Allu, S., Kalnaus, S., Simunovic, S., Nanda, J., Turner, J.A. and Pannala, S. A three-dimensional meso-macroscopic model for Li-Ion intercalation batteries. Journal of Power Sources (2016) 325 :42-50.

14th U.S. National Congress on Computational Mechanics
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Title: Face Stability Analysis in Mechanized Tunnelling: A Novel FE Approach Based on Incompatible Modes and Strong Discontinuity Kinematics

Author(s): *Abdullah Alsahly, Gunther Meschke, *Ruh University Bochum*; Callari Carlo, *University of Molise*.

During tunneling, in particular in densely populated urban areas, the assessment of the level of safety against soil collapse is crucial for the control of the construction procedure. In case of mechanized tunneling in soft soil conditions, the stability of the tunnel face depends on the level of support pressure at the cutting face, the advancement speed and stand up time. Numerical methods for predicting potential collapse mechanism due to insufficient support of the tunnel face are therefore indispensable in case of urban tunneling and complex geotechnical situations. Among computational approaches for predicting localized shear failure in elasto-plastic solids, the so-called “embedded” strong discontinuity method is often successfully used to simulate the post-localization response with negligible dependence on the finite element discretization. However, the employed discontinuity tracking strategy plays a crucial role and poses significant challenges for the implementation and robustness of the simulations, which, in particular in 3D applications, still are not fully resolved. In this contribution, we propose a novel strategy for prediction of shear localization surfaces. It exploits information from the enhanced modes when using an Enhanced Assumed Strain (EAS) formulation. EAS formulations are known to perform significantly better in capturing localized shear deformations. Based on the EAS modes, a spatial scalar function is constructed with negligible computational cost, which is based on the relations between the kinematics of strong and weak discontinuities and on bifurcation analysis of the elasto-plastic soil model. This function represents the surface of potential strong discontinuity. We emphasize the global character of this proposed novel approach, as the potential discontinuity surfaces are continuous by construction through the elements. The performance of the proposed approach to shear localization analysis is demonstrated by means of a number of benchmark tests, including comparisons of model predictions with optical measurements from laboratory tests performed to investigate tunnel face stability.

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Title: Non-Linear Boundary Conditions for a More Realistic Prediction of Femoral Fracture during Side-Fall

Author(s): *Zainab Altai, Muhammad Qasim, Xinshan Li, Marco Viceconti, *Insigneo, Sheffield University*.

Introduction: Osteoporotic hip fractures carry substantial economic burden in the ageing society. While CT-based finite element models (CT/FEM) are more accurate in predicting the femur strength than the traditional clinical tools based on areal bone mineral density (aBMD), so far the accuracy of both methods to stratify retrospective patients with hip fracture is similar. Moreover, none of the CT/FEM predicted the per-trochanteric fractures observed clinically. This indicates that the boundary constraints employed in previous studies were not completely representative of the physical event of fall. The aim of this research is to investigate whether the introduction of a non-linear boundary condition could improve the stratification of patients with respect to their risk of hip fracture and the prediction of fracture site. Methods: The study was conducted on a retrospective cohort of 98 postmenopausal women: 49 with proximal femur fractures and 49 age, height and weight pair-matched controls. Proximal femur was segmented using ITK-Snap from CT scans. Segmented bone surface was meshed using Icem CFD 14.0 (Ansys Inc., PA, USA). Three different FE models were developed. The linear model was fixed distally with no-friction slider at the greater trochanter. The MPC model had a distal end connected to the knee joint centre using multipoint constraint (MPC) allowing rotation around the horizontal transverse axis. In the contact model, the no-friction slider was replaced by non-linear contact. A 1kN concentrated point load was applied to the centre of the femoral head. Maximum principal strains location under different falling directions were recorded. Minimum failure load was estimated following maximum principal strain criterion. Area under receiver operating characteristic (ROC) curve (AUC) was calculated for all the models. Results: Mean minimum failure load predicted by the MPC and the contact models was 30% less than the linear model. Contact model had the highest AUC (0.82) among all FE models, compared to 0.80 and 0.79 for MPC and linear models, respectively. Among the cohort, 72 patients were categorized with trans-cervical neck fractures, 23 with inter-trochanteric fractures and 3 with per-trochanteric fractures, which has not been predicted previously in FE studies. Conclusions: The study demonstrated that more realistic boundary conditions of the FEM can effectively improve the stratification of patients with respect to their hip fracture risk and fracture site prediction.

14th U.S. National Congress on Computational Mechanics
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Title: Numerical Modeling of Suspension Plasma Spray

Author(s): *GHOBAD AMINI, *Concordia University*.

Thermal spraying is a process in which molten and semi-molten solid particles are deposited on a substrate. In this research, a two-way Eulerian- Lagrangian approach is employed to investigate the interaction and track the spray particles in a high-energy plasma plume in order to obtain the in-flight particle characteristics including, size, velocity, and temperature. The plasma plume is a mixture of several gases subjected to the DC arc voltage fluctuation. Reynolds Stress Model is used for time-dependent simulation of the plasma gas with its surroundings. In order to simulate the droplet breakup, Kelvin-Helmholtz Rayleigh-Taylor (KHRT) breakup model is used. In addition, various sub-models are employed to resolve the collision, melting, and evaporation of particles.

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Title: Coupled Atomistics and Discrete Dislocations in 3d (CADD-3d)

Author(s): *Guillaume Anciaux, Jaehyun Cho, Till Junge, Jean-François Molinari, William Curtin, *EPFL*.

Capturing plasticity at realistic dislocation densities with high configurational complexity requires a continuum-level discrete dislocation dynamics (DDD) description. However, many features controlling dislocation motion are inherently atomistic, such as the interaction of dislocations with solutes, precipitates, cracks, interfaces and nucleation. In two dimensions, modeling these phenomena in a multi-scale manner was possible thanks to the method Coupled Atomistic and Discrete Dislocation dynamics (CADD2d). Here, we present an approach that extends this multiscale coupling in 3d (CADD3d), while using the DDD code Paradis and the MD code LAMMPS, interfaced with the coupling code LibMultiScale. In CADD3d, dislocations can be described with atomistic resolution in one spatial domain that is fully and intimately coupled to a surrounding continuum domain in full 3d, with individual dislocation lines spanning both domains simultaneously. Having hybrid dislocations, partially represented with dislocated atoms and partially as discrete lines is a major difficulty of the presented strategy. The need for precise matching of continuum dislocation properties to atomistic dislocation properties is demonstrated, and issues in making this connection are also discussed. In particular, the dynamics of a single hybrid dislocation and of a hybrid dislocation loop, will illustrate the potential and robustness of the approach for near-seamless motion of dislocations into, across, and out of the atomistic domain. Furthermore, we present the nucleation of dislocation loops emitted from a Frank-Read source and then transformed into DD dislocations, demonstrating the possibilities of our framework.

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Title: Isogeometric Structural Shape Optimization using Bézier Triangles

Author(s): Jorge López, *Cosmin Anitescu, Navid Valizadeh, *Bauhaus-Universität Weimar*; Timon Rabczuk, *Ton Duc Thang University*.

A method for shape optimization using Bézier triangles [1] is presented. The proposed procedure takes as input a CAD-compatible boundary representation of the initial domain and outputs an optimal design while maintaining an exact geometry representation at each iteration. It also avoids some of the ill-conditioning and stability problems commonly encountered in level-set and other implicit boundary representation methods. The use of a triangular discretization allows the modeling of complex geometric domains, including voids, using a single patch. Some topology changes, such as those resulting from merging boundaries, can also be easily considered. A gradient-based optimization algorithm (the method of moving asymptotes) is employed together with a sensitivity weighting procedure. This method results in a fast convergence to the optimal shape while considering only the design variables in the original model. We apply the method to some standard benchmark problems commonly considered in the literature and show that the proposed method converges to an optimal shape in only a few iterations. Moreover, because of the higher-order (cubic) polynomials used, good results are obtained on relatively coarse meshes and without significant mesh dependency. References [1] L. Engvall, J. A. Evans, Isogeometric triangular Bernstein–Bézier discretizations: Automatic mesh generation and geometrically exact finite element analysis, Computer Methods in Applied Mechanics and Engineering, Volume 304, 1 June 2016, Pages 378-407

14th U.S. National Congress on Computational Mechanics
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Title: A Local Crack-Tracking Strategy to Model Three-Dimensional Crack Propagation with Embedded Methods

Author(s): *Chandrasekhar Annavarapu, Randolph Settgast, Efrem Vitali, Joseph Morris, *LLNL*.

We develop a local, implicit crack tracking approach to propagate embedded failure surfaces in three-dimensions. We build on the global crack-tracking strategy of Oliver et al. (Int J. Numer. Anal. Meth. Geomech., 2004; 28:609–632) that tracks all potential failure surfaces in a problem at once by solving a Laplace equation with anisotropic conductivity. We discuss important modifications to this algorithm with a particular emphasis on the effect of the Dirichlet boundary conditions for the Laplace equation on the resultant crack path. Algorithmic and implementational details of the proposed method are provided. Finally, several three-dimensional benchmark problems are studied and results are compared with available literature. The results indicate that the proposed method addresses pathological cases, exhibits better behavior in the presence of closely interacting fractures, and provides a viable strategy to robustly evolve embedded failure surfaces in 3D.

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Title: An Adaptive Approach with Local Reduced Basis Approximation for the Solution of PDEs with Uncertain Inputs

Author(s): Zilong Zou, *Wilkins Aquino, *Duke University*.

Uncertainty is ubiquitous in virtually all engineering applications and, for such problems, it is inadequate to simulate the underlying physics without quantifying the uncertainty in unknown or random inputs, boundary and initial conditions, and modeling assumptions. Additionally, when solving partial di erential equations (PDEs) with random inputs, it is often computationally inefficient to merely propagate samples of the input probability law (or an approximation thereof) because the input law may not accurately capture the behavior of critical system responses that depend on the PDE solution. In this work, we develop an efficient method for approximately solving PDEs with random inputs. Our method employes a local reduced basis method in conjunction with an adaptive sampling procedure. In the method, we adaptively determine a set of parameter atoms and an associated (implicit) Voronoi partition of the parameter domain on which we build local reduced basis approximations of the PDE solution. The parameter atoms are selected in a sequential and greedy manner according to an a posterior error indicator. We provide theoretical error bounds for our approximations and employ several numerical examples to showcase the efficacy of our method.

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Title: The Discontinuity-Enriched Finite Element Method (DE-FEM)

Author(s): *Alejandro M. Aragón, Angelo Simone, *Delft University of Technology*.

We introduce a new methodology for modeling problems with both weak and strong discontinuities independently of the finite element discretization. At variance with the eXtendend/Generalized Finite Element Method (X/GFEM), the new method, named the Discontinuity-Enriched Finite Element Method (DE-FEM), adds enriched degrees of freedom only to nodes created at the intersection between a discontinuity and edges of elements in the mesh. In this presentation we show several features of the method. Firstly, DE-FEM converges at the same rate than the standard FEM with meshes that match the cracked geometry. Secondly, we show the capability of the method in extracting stress intensity factors. Lastly, we focus on the conditioning of the method and compare it with that of XFEM/GFEM.

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Title: Grain Boundary Structural Phase Transition under Mechanical Loading in Cu

Author(s): *Mohammad Aramfard, Chuang Deng, *University of Manitoba*.

Grain boundary structural transition has prominent influence on many properties of polycrystalline materials specially in nanocrystalline metals. While structural and phase transition in multi-component systems is common and phase diagrams are available for many alloy systems, reports on phase transition in single-component systems specially at low dimensions such as grain boundary are rare due to experimental challenges. Phase transformation in grain boundaries and its underlying mechanisms therefore remain unclear and are not well studied until a few recent attempts based on atomistic simulations. In this talk, we report systematic study on phase transitions of a few types of high-angle symmetric tilt grain boundaries based on molecular dynamics simulations by using Cu as a model system. The focus was to investigate the possible influences of two types of loading, i.e. creep and fatigue, on grain boundary structural transition. One potential application of the grain boundary structural transition on crack healing is also demonstrated, which is facilitated by shear coupled grain boundary motion.

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Title: Optimization of Framed Structures Subjected to Blast Loading

Author(s): Mustafa Al-bazoon, *Jasbir Arora, *The University of Iowa*.

In this study, optimum design of three-dimensional braced steel structures subjected to blast loading is considered. The optimization problem is to minimize the total weight of the structure subjected to American Institute of Steel Construction (AISC) strength requirements, geometrical limitations, and displacement constraints. The design variables for beams, columns, and bracing are the discrete values for the W-shapes selected from the AISC tables. Layout of the bracing system is also considered as a design variable. A car carrying 100 lbs of TNT with 100 ft. standoff distance at three locations of the structure is modeled as the source of the blast loading. Each side of the structure is divided into panels and the reflected pressures calculated at the panel's center are then distributed to the beams and columns uniformly. The formulation of this optimization problem has discrete design variables. In addition, the strength constraints based on the AISC Manual have discontinuities at some points. Therefore they are nondifferentiable. Thus the traditional gradient-based optimization algorithms are not applicable to this problem. Therefore nongradient-based optimization methods, such as harmony search and colliding bodies optimization algorithms are used to solve the problem. The optimization algorithms are coded in MATLAB® and interfaced with the structural analysis program SAP2000 using the Open Application Programing Interface. Example problems are solved to study the formulation of the optimization problem and its final solutions. The problems are 4-bay x 4-bay x 2-story frames under service and blast loading conditions with and without horizontal and vertical braces. It is shown that with appropriate bracing it is possible to design minimum weight structures to withstand the blast loading. Also it is seen that a feasible design for the structure cannot be obtained without a bracing system. Principal contributions are the optimization problem formulation and its solution process. Outline of Presentation 1. Introduction 2. Review of Literature 3. Optimal Design Problem Formulation 3.1 Design Variables 3.2 Cost Function 3.3 Constraints 4. Blast Loading 5. Optimization Algorithms 6. Numerical Examples 6.1 Four-bay Two-story 3D Frame without Braces. 6.2 Four-bay Two-story 3D Frame with Braces. 7. Conclusions References Degertekin S. O., (2008). Optimum design of steel frames using harmony search algorithm. Struct Multidisc Optim 36:393-401. U.S. Department of the Army, (1990). Structures to resist the effects of accidental explosions. Technical Manual 5-1300.

14th U.S. National Congress on Computational Mechanics
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Title: GraFEA: A Graph Based FEA to Study Damage in Brittle Materials

Author(s): Parisa Khodabakshi, *Texas A&M University* ; Junuthula Reddy, *Srinivasa Arun, *Texas A&M University*.

We present a novel graph-based finite element framework (GraFEA) suitable for the study of damage in brittle materials. GraFEA stems from conventional finite element method (FEM) by transforming it to a network representation (Reddy and Srinivasa,Finite Elements in Analysis and Design, 104:35-40,2015, Khoadbakshi, Reddy and Srinivasa,Meccanica, 51(12):3129-3147, 2016) wherein forces and strains are directed only along the edges of the elements of the discretized continuum. This surprising result stems from the translational and rotational invariance of classical mechanics. The resulting model shows that any conventional FEM can be converted into a truss-like network with one essential distinction: In the network representation of GraFEA the magnitude of the force along each edge depends on the collective behavior of the strains along the neighboring edges, and not only on the strain along that specific edge. The network representation of GraFEA allows for the implementation of an edge-based failure criterion which is based on the idea of weakest link statistics introduced by Lin, Evans, and Ritchie Journal of the Mechanics and Physics of Solids, 34(5):477-497, 1986). If the strain along an edge (calculated as a weighted average across a characteristic zone) exceeds a critical strain, the edge is considered broken and the crack passes through that edge. These unique features of GraFEA makes it appealing for the study of damage in solids. As opposed to the continuum-based approaches to damage and fracture GraFEA handles damage in a discrete way thus eliminating the need for shape function augmentation. Furthermore, the ability to impose an edge-based failure criterion in GraFEA is similar to the existing discrete methods (e.g. lattice models and bond based peridynamics), yet GraFEA doesn't suffer from limitations such as those related to Poisson's ratio. P. Khodabakhshi, J. N. Reddy, and A. R. Srinivasa. GraFEA: a graph-based finite element approach for the study of damage and fracture in brittle materials. Meccanica, 51(12):3129{ 3147, 2016. [2] J. N. Reddy and A. R. Srinivasa. On the force-displacement characteristics of finite elements for elasticity and related problems. Finite Elements in Analysis and Design, 104:35{40, 2015. [3] T. Lin, A. G. Evans, and R. O. Ritchie. A statistical model of brittle fracture by transgranular cleavage. Journal of the Mechanics and Physics of Solids, 34(5):477 { 497, 1986.

14th U.S. National Congress on Computational Mechanics
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Title: Capabilities of Shallow Water Equations to Reproduce Real Tsunamis, Cases of Tohoku 2011 and Gisborne 1947

Author(s): Marine Le Gal, *Saint-Venant Lab.* ; *Riadh Ata, Damien Violeau, *EDF-LNHE-LHSV*.

Shallow water equations are the most used model to simulate real cases of tsunamis. Their use is mainly justified by their relative low computational cost compared to other more complex models. Even though these equations are non-dispersive, they can reproduce accurately both wave heights and arrival times. Moreover, they are well suited for the simulation of flooding of coastal areas with the help of nested or full extended models (meshes containing oceanic and flooded coastal areas). Dispersive models, such as Boussinesq or Navier-Stokes, can be with a prohibitive cost and with less attractive numerical properties. In this talk we give a simple and direct way to identify a priori whether Saint Venant equations are able or not to tackle a tsunami case. This approach is based on linear theory and on the definition of an energy ratio [1]. This approach is applied on two real cases, the tsunamis of Gisborne 1947 and Tohoku 2011. The open source Telemac-2D code [2] is used to simulate the propagation and flooding of coastal region. A comparison with a Boussinesq model is also presented.

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Title: Bayesian Deep Gaussian Processes for Nonlinear Stochastic Dimensionality Reduction

Author(s): *Steven Atkinson, Nicholas Zabaras, *University of Notre Dame*.

The Bayesian deep Gaussian process (DGP) model has recently emerged as an attractive framework for constructing surrogate models for complex physical processes that are prohibitive to study directly through high-performance simulation codes [1]. However, the tool is still in its early stages and many potential applications exist within the field of UQ that merit investigation. Here, we discuss the application of our fully Bayesian extension of the recently-developed unsupervised DGP framework [2] as a generative model for nonlinear dimensionality reduction and hierarchical feature representation. This tool may be fruitfully applied to systems possessing high-dimensional stochastic inputs that are inhibitive to handle directly in UQ contexts. Typically, one might search for some reduced-dimensional representation (such as a Karhunen-Loeve expansion) that reflects the correlations in the raw inputs. Unlike many standard methods, the unsupervised DGP is built on a fully Bayesian framework that allows for the rigorous propagation of uncertainty which is of critical importance in UQ. Additionally, we will discuss the merits of the DGP's generative nature which allows one to propagate new samples back and forth between the learned latent space and the observed stochastic space. Finally, we will demonstrate how one may incorporate the results of the unsupervised dimensionality reduction to perform standard UQ tasks, using the problem of flow through porous media for demonstration. [1] S. Atkinson and N. Zabaras (2017), in progress [2] A. C. Damianou and N. D. Lawrence, Deep Gaussian Processes, AISTATS (2013)

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Title: A CFD Study of Supercooled Cloud Size Droplet Impact on a Superhydrophobic Surface

Author(s): *Reza Attarzadeh, Firoozeh Yeganehdoust, Ali Dolatabadi, *Concordia University*.

Supercooled Liquid Droplets (SLD) are the main components of cold clouds and their impact is a well-known phenomenon in atmospheric physics and aeronautics. Most of the ice accretion on critical aerodynamic surfaces is due to the impact of supercooled droplets which aircrafts frequently pass through during take off and landing. Because of the rapid solidifcation of supercooled droplets, aircraft icing is a safety hazard issue in aerospace engineering. Recently significant effort has been dedicatd to assess the applicability of superhydrophobic coatings to repel water droplets to prevent icing problem. The focus of this study is to simulate cloud-sized supercooled droplets impacting on a textured superhydrophobic surface to predict the onset of freezing. A multi-region solver including free surface, phase change, and conjugate heat transfer at liquid-solid interface has been employed to model the icing of a super- cooled micro-droplet as it impinges on a textured superhydrophobic surface with a given thickness, morphology, and material. The Navier-Stokes equation expressing the ow distribution of the liquid and the gas, coupled with the volume of fluid (VOF) method for tracking the liquid-gas interface, was solved numerically using the finite volume methodology. A dynamic contact angle model is applied as a boundary condition at liquid-solid contact lines. Heat transfer within the substrate was solved solely by conduction and the momentum/energy equations in both the liquid and solid portions of the droplet are solved using the modified formulation. The freezing model is based on the nucleation theory, making use of Gibbs free energy as a trigger for instantaneous freezing of supercooled upon contact with the surface. Hence, no adjusting parameter was used for the freezing front of the supercooled droplet. In order to simulate the in-fight condition, a supercooled droplet with a size of 20 _m is impinged on a superhydrophobic surface. The superhydrophobic surface topology is modeled through series of micro-structured pillars. Consequently, direct effect of surface topology and thermal properties on droplet maximum spreading diameter, penetration to the surface asperities, contact time, and freezing time have been investigated. Based on different supercooling temperature, different outcome has been observed; sticky, partial sticky with solidified residual on the surface and complete detachment. It was observed that surface asperities decrease the interface temperature due to low thermal conductivity of entrapped air. The results can be used to identify critical properties required by an icephobic coating to prevent the onset of ice formation under in-fight icing condition.

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Title: Hydrodynamic Coupling Within Curved Lipid Bilayer Membranes: The Role of Curvature in the Drift-Diffusion Dynamics of Proteins

Author(s): *Paul Atzberger, Ben Gross, *University of California Santa*.

We presents results on the importance of geometry and topology in hydrodynamic responses associated with lipid flow and the drift-diffusion of protein inclusions within curved lipid bilayer membranes. In 1975, Saffman and Delbruck introduced a hydrodynamic theory for infinite flat sheets that is still widely used to investigate membrane protein diffusivity. We find that for curved lipid bilayer membranes new phenomena emerge that significantly augment hydrodynamic flows and the predictions of the classical Saffman and Delbruck theory. For bilayer vesicles we explore both the role of topology and geometry on the individual and collective responses of embedded proteins. We find that local variations in the Gaussian curvature can significantly change hydrodynamic flows through increased local dissipation. This leads to interesting new patterns in the flow and coupling between protein inclusions. We develop our theory and computational methods based on the exterior calculus of differential geometry to take into account the hydrodynamics within curved leaflets of the membrane, intermonolayer slip between the leaflets, and coupling with the surrounding bulk solvent fluid. We present our results showing how these effects contribute to the hydrodynamic flows within vesicles having different shapes. We then develop fluctuating hydrodynamic methods for manifolds and show how the geometry and topology of curved vesicles impact the drift-diffusion dynamics of protein inclusions. We then discuss ways these effects could be used in lipid membranes to augment protein kinetics.

14th U.S. National Congress on Computational Mechanics
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Title: Boundary Layer Mesh Generation

Author(s): *Romain Aubry, *U.S. Naval Research Laboratory*.

Boundary layer mesh generation is still a challenge for complex three dimensional geometries. For surfaces, we have shown that a very limited set of capabilities seems to be able to provide predictability, robustness and accuracy. These capabilities have been recently applied to three dimensional boundary layer volumes and seem to provide in practice enough guidance to generate reliable and accurate boundary layer meshes.

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Title: A Computational Heart Model of Pulmonary Arterial Hypertension

Author(s): *Reza Avazmohammadi, Emilio Mendiola, Joao Soares, Michael Sacks, *The University of Texas at Austin*; Richard Dixon, *Texas Heart Institute at Houston*.

Pulmonary arterial hypertension (PAH) imposes a pressure overload on the right ventricular free wall (RVFW), leading to substantial growth of muscle cells and remodeling in fiber architecture [1]. The effects of these alterations on the biomechanical behavior of the RVFW and the organ-level cardiac function remain largely unexplored. A recent study [1] on the mechanical and morphological properties of normal and hypertensive RVFW myocardium strongly suggest that myocardial wall stress is the primary mediator of RVFW growth and remodeling (G&R) responses. An accurate quantification of the wall stress evolution during the development of PAH is needed to determine the correlation between the wall stress and G&R mechanisms. To this end, there is a need to develop a detailed computational heart model [2] that can accurately simulate the effect of PAH in the heart, and thus can be used to understand pathophysiology of RVFW remodeling, its connection to wall stress alterations, and its impact on organ-level cardiac function. We have developed a high-fidelity finite-element (FE) heart model of PAH using extensive time-course datasets from a normal rat heart and from a hypertensive rat heart simulating the pressure overload in the right ventricle (RV). We built on open-source packages in FEniCS, and developed a pipeline that integrates a meshed geometry from a high-resolution image of the rat heart, detailed imaging data on the fiber structure of the same heart, and a novel compressible hyperelastic material model accounting for both passive and active behaviors of myocardium. The developed heart model within the FEniCS environment together with the Python interface offer a high performance capability for inverse problems requiring the simultaneous conduct of a large number of forward simulations such as fine-tuning the active properties of myocardium or characterizing shape change patterns of the RV. We used our model to investigate the correlations between the alterations in the wall stress, the remodeling of the RVFW microstructure, and the shape changes in the RV during the development of PAH. The detailed description of organ-level remodeling patterns can replace the traditional measures of RV dimensions and volume that often lead to gross and limited information on cardiac performance. Ultimately, development and implementation of our model in patient-specific organ-level simulations will allow investigation of optimal diagnosis and new individualized stem-cell interventions for PAH. References: [1] Avazmohammadi, Reza, et al. Biomechanics and Modeling in Mechanobiology (2016): 1-21. [2] Chabiniok, Radomir, et al. Interface focus 6.2 (2016): 20150083.

14th U.S. National Congress on Computational Mechanics
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Title: The Adaptive Wavelet Enhancement of the Crystal Plasticity Finite Element Method

Author(s): *Yan Azdoud, *Johns Hopkins University*; Jiahao Cheng, Somnath Ghosh, *Johns Hopkins University*.

The simulation of Crystal Plasticity based on realistic heterogeneous microstructure is computationally challenging. This is a consequence of the high number of degrees of freedom necessary to accurately capture local behavior. Providing an efficient discretization method, which follows the evolution of the plastic behavior is, therefore, paramount. The adaptive wavelet enhancement simulation method is proposed to overcome these challenges. Recently, Fast Fourier Transform based method have been proposed for the simulation of Crystal Plasticity, as an alternative to Finite element methods. While being fast for a given resolution, such methods are restricted to periodic structures and show low convergence rates for discontinuous, heterogeneous materials. Hence, we propose a more general approach which extends the conventional FEA framework. This method is a new paradigm for adaptive enrichment which replaces the typical error indicator/ mesh subdivision scheme by a solution estimate/ optimal discretization selection method. In this method, a computationally cheap solution estimate is first computed, which is then decomposed using a wavelet transform to identify an optimal base of hierarchical discretization enrichment functions, on which an FEA solution can be sought. The new method improves the convergence rate of the solution and is computationally less costly for large problems. A comparative study between FFT and FEM strategies is presented to justify our approach. The implementation of the Adaptive Wavelet Enhancement method is discussed in Crystal Plasticity. The efficiency of the method is demonstrated on a polycrystalline crystal plasticity example.

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Title: Gradient-Based Optimization Algorithms for the Modified Error in Constitutive Equation Approach to Inverse Problems

Author(s): *Olalekan Babaniyi, Clay Sanders, Wilkins Aquino, *Duke university*.

We will discuss our current work on reduced-space Modified Error in Constitutive Equations (MECE) formulations for materials characterization in inverse elastodynamics problems. Our previous work on MECE has exclusively employed alternating directions algorithms to search for minimizers. The latter approach, despite showing robustness in practice, is just linearly convergent, which can be too slow in many practical cases. Therefore, with the goal of accelerating convergence near minimizers, we now incorporate Hessian and gradient information of the MECE reduced objective function within trust region or line search algorithms. Moreover, we will present studies on the eigenspectrum of the Hessian at optimality that provide insight into the stability of minimizers in MECE formulations. We will illustrate our findings through numerical examples drawn from frequency-domain elastodynamics inverse problems.

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Title: A Saddle Point Least Squares Method for First Order Systems

Author(s): *Constantin Bacuta, Klajdi Qirko, *University of Delaware*.

We introduce a Saddle Point Least Squares method for discretizing first and second order boundary value problems written as primal mixed variational formulations. For the mixed formulation we assume a stability LBB condition and a data compatibility condition at the continuous level. For the proposed discretization method a discrete $\inf-\sup$ condition is automatically satisfied by the natural choices of test spaces (first) and the corresponding trial spaces (second). The discretization and the iterative approach does not require nodal bases for the trial space and a preconditioner acting on the discrete test space can be adopted to speed up the approximation process. A stopping criterion based on matching the order of the the iteration error with the the order of the expected discretization error is considered. Applications of the method include discretizations of second order PDEs with oscillatory or rough coefficients and first order systems of PDEs, such as $div-curl$ systems and time-hamonic Maxwell equations.

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Title: Unstructured All-Quadrilateral Mesh Generation on Complicated 3D Surface

Author(s): Zihao Zhu, *James Baeder, *University of Maryland*.

HAMSTR is a newly developed flow solver that utilizes Hamiltonian paths and strand grids for three-dimensional flows on overset and hybrid meshes. In order to use HAMSTR, it is required that one has a decent unstructured surface mesh as well as surface normal vector; this is the motivation for the development of HAMSTRAN. It is an indirect method to create an unstructured all-quadrilateral 3D surface mesh. It transforms triangular as well as quad-dominant surface meshes into all-quad meshes, without any smoothing post-processing steps. The proposed method is fast and can work on highly complicated surfaces with lots of sharp features while keeping the number of irregular grid points low. HAMSTRAN is mostly based on the Q-Tran algorithm, but it has many advantages over Q-Tran. For example, the Q-Tran algorithm can create loopholes when implemented in complicated surfaces and it can only accept an all triangular mesh as background mesh. HAMSTRAN is not only able to utilize an all-triangular mesh, but can also use quad-dominant and hybrid meshes as input and generate a decent all-quad mesh without any of the loopholes. HAMSTRAN not only preserves the vertices of the input tessellation, it also flushes the newly generated vertices onto the surface, making sure the quad mesh represents the surface features of the geometry. After creating the surface mesh, HAMSTRAN proceeds to create the normal vectors for each vertex. The vectors extrude from the surface in the wall-normal direction without crossing each other. The direction of the vectors can be adjusted according to the 3D volume mesh required for the future flow solving process. Several examples will be presented to demonstrate the efficiency of this method, such as for airfoils, wings, rotor blades and fuselage.

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Title: Computational Analysis of the Process of Metal Material Free-Surface Instability, Fragmentation, and Ejecta under Shock

Author(s): *Jingsong Bai, *Institute of Fluid PhysicsCAEP*.

We conducted numerical simulations of the related processes of interface instability, tensile fragmentation, and jetting resulting from four kinds of typical macro defect perturbations (chevron, sine wave, rectangle, and square) on a Cu free surface under a reflected shock wave when Cu impacts a solid wall at a speed of 2.5 km/s and found that, for the chevron and sine wave cases, the ejecta velocities of the head are 6.28 and 5.88 km/s, respectively. Some parts of the inner material are in a tensile state without any fragmentation, which is observed only in the main body of the material owing to the tension effect. Furthermore, for the other two initial perturbations (rectangle and square), the highest ejecta velocities may even reach 9.14 and 9.59 km/s, respectively. Fragmentation caused by multilayer spallation can be observed on a large scale in the Cu main body, and there are granules in the front area of the ejecta but the degree to which fragmentation occurs is much less in the Cu main body and there is a notable high-speed, low-density granule area in the ejecta head. Finally, we present a detailed analysis of the spatial distribution of the granules, ejecta mass, pressure, temperature, and grid convergence.

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Title: Deforming Grid Method for Dimensionality Reduction of Convection Dominated Nonlinear Flows

Author(s): *Maciej Balajewicz, *University of Illinois*.

I will discuss a new projection-based model order reduction approach specifically tailored for solutions characterized by traveling waves, moving shocks, sharp gradients and discontinuities. In this new approach, the reduction is performed in a arbitrary Lagrangian-Eulerian frame of reference. That is, global basis functions are used to approximate both the state and the coordinates of a deforming computational grid. It is demonstrated that in this framework, certain wave-like solutions exhibit low-rank structure and thus, can be efficiently compressed using a relatively small number of global bases.

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Title: Current Efforts in Developing an Optimum Biaxial Tensile Test Specimen Design

Author(s): *Dilp Banerjee, Mark Iadicola, Adam Creuziger, Evan Rust, *NIST*.

Traditional uniaxial tensile test data are not easily applicable in the multidirectional forming processes involving nonlinear strain paths as sheet metals have highly anisotropic properties. Biaxial tensile tests are commonly used for developing mechanical properties of sheet metals. However, there are major challenges in developing an optimum test specimen design. Current approach of developing an optimum biaxial specimen design combines optimization software with a verified finite element analysis (FEA) model. The FEA model is verified against time-dependent, measured displacement and strain fields obtained during controlled, biaxial tensile test experiments conducted on steel specimens with an initial specimen design. Constitutive material property data for these AISI 1008 steel specimens are developed through controlled uniaxial tests conducted at various average strain rates. The optimization technique uses several numerical techniques and different objective functions along with proper design variables and constraints to arrive at an optimum design. Finally, a specimen is fabricated with optimum values of critical design parameters and measured strain and displacement data in the gauge section obtained from test on this specimen are compared with the optimum FEA model predictions to demonstrate the efficacy of the overall methodology used.

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Title: A Stable Partitioned FSI Algorithm for Rigid Bodies and Incompressible Flow

Author(s): *J. W. Banks, W. D. Hensahw, D. W. Schwendeman, Q. Tang, *Rensselaer Polytechnic*.

This talk will discuss a stable partitioned algorithm for fluid-structure interaction problems involving viscous incompressible flow and rigid bodies. This added-mass partitioned (AMP) algorithm remains stable, without sub-iterations, for light and even zero mass rigid bodies when added-mass and viscous added-damping effects are large. The scheme is based on a generalized Robin interface condition for the fluid pressure that includes terms involving the linear and angular acceleration of the rigid body. Added mass effects are handled in the Robin condition by inclusion of a boundary integral term that depends on the pressure. Added-damping effects due to the viscous shear forces on the body are treated by inclusion of added-damping tensors that are derived through a linearization of the integrals defining the force and torque. Added-damping effects may be important at low Reynolds number, or, for example, in the case of a rotating cylinder or rotating sphere when the rotational moments of inertia are small. Here we begin by discussing the development and analysis of the AMP scheme for simple model geometry. Extension of the scheme to general geometry is then performed using finite difference methods and overlapping grids. Stability for light solids, and second-order accuracy are demonstrated for a series of challenging benchmark problems.

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Title: High-Performance Computing in the Modeling of Hydraulic Fracturing

Author(s): *Denis Bannikov, Alexey Tikhonov, Vadim Isaev, Ivan Velikanov, Dmitry Kuznetsov, *Schlumberger*.

Field use of fine-scale hydraulic fracturing simulators is strictly limited due to a long computational time. Application of high-performance computing (HPC) tools significantly accelerates the simulation, thereby enabling the use of the simulators for the design of real treatments. A modern fracturing simulator is a complex system comprising numerous components. We will present our experience in the application of HPC tools for some critical components affecting the overall algorithm performance: pressure solver, transport algorithm, etc. Areas considered are the capabilities of modern languages (Fortran and C++), parallel computing tools (OpenMP, OpenACC, CUDA, and MPI), hardware (CPU and GPU), and efficient formats for data input and output. Organization of the development process of a fracturing simulator has a strong effect on the quality. We will share our experience in the waterfall approach, test-driven development (TDD), and prototyping. Numerous high-quality fracturing codes were created in the past. We will discuss various aspects related to the use of legacy code. Finally, the capabilities offered by the application of HPC tools in hydraulic fracture modeling will be demonstrated in case studies.

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Title: Inverse Problems in Highly Heterogeneous Media

Author(s): *Paul E. Barbone, *Mechanical Engineering, BU*; Danial Panahandeh, Bojan Guzina, *Civil, Env, & Geo Eng, UMN*.

Full-field data of deformation fields is becoming widely available. From such full-field data, an inverse problem for the material properties at the scale of the observation can be formulated and solved. It is often the case, however, that additional length scales are inherent in the data, arising from either the material properties themselves or from the deformation field (e.g. a wavelength). It is of interest, therefore, to understand the interplay between these different length scales and thus to understand the role of the observation length scale on the properties observed and reconstructed. We study this issue through a series of both forward and inverse model problems. The forward problems provide high resolution elastic wavefields in media with microstructure. We then apply an observation operator (i.e. a smoothing operator) with a defined spectral structure to obtain simulated “measured” data. We model measurement error using additive noise. Using these data, we reconstruct the effective material property distributions as a function of observation scale, and compare these to the effective material properties as predicted by asymptotic homogenization theory [1]. The results have implications on the interpretation of effective material properties, and also on the ability to infer microstructural quantities from macroscopic observations [2]. [1] Wautier, Antoine and Guzina, Bojan B. On the second-order homogenization of wave motion in periodic media and the sound of a chessboard. Journal of the Mechanics and Physics of Solids 78 (2015) 382–414. [2] Liu, Tengxiao, Timothy J. Hall, Paul E. Barbone, and Assad A. Oberai. Inferring spatial variations of microstructural properties from macroscopic mechanical response. Biomechanics and Modeling in Mechanobiology (2016): 1-18.

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Title: A Bounding Surface Plasticity Model For Natural Clay – Calibration, Validation and Application

Author(s): *Thomas Barciaga, Tom Schanz, *Ruhr-Universität Bochum*.

Reliable predictions of the system response of geotechnical applications in natural clay deposits such as cyclic stress-induced ground movements and time-dependent consolidation processes are demanding due to the complex constitutive behavior of natural clay. Therefore, it is essential to employ constitutive models accounting for the behavior of natural clay which is governed by state, cyclic stress-strain history and structure. The structure of natural clay is composed of the fabric referring to the arrangement and the orientation of the particles and contacts and the interparticle bonding. Fabric is related to an inherent or stress-induced anisotropy with respect to the mechanical properties of the clay. Bonding imparts additional strength and stiffness to the clay compared to its intrinsic properties. After exceeding the yield stress clay will experience a destructuration process where the bonding will be progressively destroyed. Within this study an adequate hierarchical constitutive soil model based on the bounding surface plasticity (BSP) concept is employed. Inherent and stress-induced anisotropy is considered by a fabric tensor whose evolution is controlled by a sophisticated rotational hardening rule. A structure parameter is introduced to account for the current amount of structure by relating the size of the yield surface of the natural clay to the size of a reference surface of the corresponding reconstituted clay. The destructuration process and hence the evolution of the structure parameter is governed by the evolution of the plastic strains. The BSP concept allows for a smooth elasto-plastic transition and the accumulation of plastic strains with respect to cyclic loading. In order to calibrate the constitutive parameters and validate the constitutive model geotechnical experiments are numerically simulated considering natural and reconstituted state, isotropic and anisotropic consolidation, monotonous and cyclic loading and drained and undrained hydraulic conditions. Sensitivity of the model responses of geotechnical element tests to the constitutive model parameters of the BSP model is investigated using global sensitivity analysis. As application case, the model is tested against mechanized tunneling induced ground movements. Mechanized tunneling in natural clay deposits is challenging due to the complex hydro-mechanical interactions between soil, tunnel boring machine (TBM), lining and support materials resulting in non-monotonous loading and consolidation in the near-field around the TBM. The hierarchical structure of the constitutive model allows for the investigation of the necessity of the model complexity level with respect to a certain model response in mechanized tunneling such as ground movement, excess pore-water pressures, lining forces and moments.

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Title: Transparent Performance Monitoring for Engineering Computation

Author(s): *William Barth, Todd Evans, *TACC*.

High-performance computing systems comprise a complex array of processors, memory, networks, storage systems, and hardware. Users and managers of these systems are faced with uncertainty in understanding if systems are being used optimally or even if all subcomponents are functioning properly. This talk presents the results of ongoing work to transparently monitor and collect relevant performance data and metadata about these systems and their use. These results include the automated identification of workloads requiring investigation from the Stampede supercomputing cluster at the Texas Advanced Computing Center and the outcome of interventions with the users who initiated these workloads.

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Title: Data-Driven Modeling of Turbulent Boundary Layer Noise

Author(s): *Gregory Bartram, *Universal Technology Corporati*.

To study the fine details of fluid-structure interactions, recent advances in full-field measurement techniques such as 3-D digital image correlation (DIC) and pressure sensitive paint (PSP) have been implemented by researchers at Wright-Patterson Air Force Base. These techniques collect spatially dense data using high speed cameras, yielding large volumes of high-dimensional data. Models of such data enable simulation of experimental conditions, potential extrapolation to new conditions, and deeper study of the problem domain. However, high dimensionality often renders first principles models, or even data-driven models, too costly to calibrate/train and evaluate. A good model is efficiently trained and evaluated, despite the data's dimensionality and correlations, while being accurate. To efficiently model turbulent boundary layer noise from PSP measurements, a data-driven modeling approach based on Devathi et al. [1] and da Silva et al. [2] is employed. Singular value decomposition (SVD) transforms the data into many uncorrelated variables, changing the modeling task from training one high dimensional model to making many univariate models. Further, SVD facilitates extracting structurally relevant components from the multiscale pressure field. Autoregressive (AR) models are then fit to the transformed data due to their ability to efficiently and accurately model the time and frequency components of the data without requiring any knowledge of the physics. Data simulated by the AR models is easily rotated back to the original problem space. Current quantitative validation results demonstrate agreement in the time, space, and frequency domains. This indicates that the SVD+AR approach has scaled up well, from modeling tens of variables in Devathi et al. [1] and da Silva et al. [2] to thousands of variables of the PSP data. Future SVD+AR applications include additional study of PSP and DIC datasets to isolate features of fluid-structure interactions, as well as exploring other high dimensional datasets. References: [1] Devathi, H., Hu, Z., and Mahadevan, S., "Snap-Through Buckling Reliability Analysis Under Spatiotemporal Variability and Epistemic Uncertainty," AIAA Journal, vol. 54, 2016, pp. 3981–3993. [2] da Silva, S., Dias Júnior, M., Lopes Junior, V., and Brennan, M. J., "Structural damage detection by fuzzy clustering," Mechanical Systems and Signal Processing, vol. 22, Oct. 2008, pp. 1636–1649.

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Title: An Immersed Boundary Formulation for Simulating High-Speed Compressible Viscous Flows with Moving Solids

Author(s): Yegao Qu, *Shanghai Jia Tong University*; *Romesh Batra, *Virginia Tech*.

This paper presents a robust sharp-interface immersed boundary method for numerically studying compressible, viscous and high speed flows interacting with arbitrarily shaped either stationary or moving rigid solids. The Navier-Stokes equations are discretized on a rectangular Cartesian grid based on a low-diffusion flux splitting method for the inviscid fluxes and conservative high-order central differences for the viscous components. Different discontinuities in high speed flows, such as shock waves and contact surfaces, are captured by using a high-resolution weighted essentially non-oscillatory (WENO) scheme. Ghost cells in vicinity of the fluid-solid interface are introduced to satisfy boundary conditions on the interface. Values of variables in the ghost cells are found by using a constrained moving least squares method (CMLS) that eliminates numerical instabilities encountered in the conventional MLS formulation. The solution of the fluid flow and the solid motion equations is advanced in time by using the third-order Runge-Kutta and the implicit Newmark integration schemes, respectively. The performance of the proposed method has been assessed by computing results for four problems that shock-boundary layer interaction, supersonic viscous flows past a rigid cylinder, moving piston in shock tube and lifting off from a flat surface of circular, rectangular and elliptic cylinders triggered by shock waves.

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Title: Non-Symmetrical Hydraulic Fracture Propagation Due to Poroelastic Effects

Author(s): *Alexey Baykin, *Novosibirsk State University*; Sergey Golovin, *Lavrentyev Institute of Hydrodynamics of SB RAS*.

Hydraulic fracturing is an important part of modern technologies for intensification of hydrocarbon production. The propagation of the hydraulic fracture is stimulated by the pumping of viscous fluid which creates pressure on fracture's walls high enough to overcome the rock closure stresses and cause the rock failure. In present work we investigate the symmetry of the hydraulic fracture propagation using the poroelastic model [1] extended to the case of propagating fractures. The model allows determining the porous pressure and the rock deformation coupled with the fracture width and the pressure of the fracturing fluid. The formation is regarded as an inhomogeneous permeable medium governed by Biot's equations [2]. The advantages of this approach in comparison with ones based on the elasticity theory are the correct account for the interaction of the pore fluid with the fracturing fluid, finiteness of fluid pressure in the fracture's tip, ability for modelling of reservoirs with inhomogeneous physical properties and non-uniform prestress state. The cohesive zone model [3] is adopted as a rock failure criterion. The numerical solution of the problem is carried out by the finite element method. The numerical convergence of the algorithm is verified. We thoroughly investigate the influence of the pore pressure and rock deformation on the fracture propagation and fracture geometry. In the series of numerical experiments, we demonstrate the impact of the pore pressure distribution on the fracture dynamics in the layered reservoir with permeability contrast. The simulation results are interpreted in terms of the calculated non-uniform backstress acting as an extra closure stress on the fracture walls due to fluid filtration outside the fracture. It is shown that the symmetry of fracture wings is essentially sensitive to such inhomogeneity of the poroelastic medium. The results are demonstrated in 2D, but the model can be extended to the 3D case where the qualitative conclusions will hold as well. The work is partially supported by Russian Science Foundation (project 15-11-20013). References [1] V.V. Shelukhin, V. A. Baikov, S.V. Golovin, A.Y. Davletbaev, V. N. Starovoitov Fractured water injection wells: Pressure transient analysis, Int. J. Sol. Struct. 51 (2014) 2116–2122. [2] M. A. Biot Theory of elasticity and consolidation for a porous anisotropic solid, Journal of Applied Physics. 26 (1955) 182–185. [3] G. I. Barenblatt The mathematical theory of equilibrium cracks in brittle fracture, Adv. Appl. Mech. 7 (1962) 55–129.

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Title: A Flexible FSI Framework with Applications

Author(s): *Yuri Bazilevs, *UC, San Diego*.

A flexible Fluid-Structure Interaction (FSI) framework is presented. The framework is derived on the basis of an Augmented Lagrangian formulation for FSI, and is suitable for discretizations using conforming as well as immersed approaches. Isogeometric Analysis (IGA) is an integral part of the FSI framework in that it delivers highly accurate fluid and structural mechanics solutions and provides a natural integration with geometry modeling and computer-aided design. The presentation is infused with a variety of FSI simulations stemming from advanced engineering applications and ranging from floating offshore wind turbines to air-blast-structure interaction.

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Title: Cavitation Bubble Effects on Cell Disruption via Shockwave Modeling

Author(s): *Matthew Becton, Xianqiao Wang, *University of Georgia*.

With current soft matter technology, designed lipid structures are able to accomplish sensitive tasks such as binding selected surfaces, serving as catalytic nanoreactors for controlled chemical reactions, dispersing CNTs into solution, and the carrying and delivering drugs or other payloads into cell interiors. Studies have shown that ultrasound can be used to destroy drug-carrying liposomes to release their payloads; however, a shockwave energetic enough to rupture lipid membranes can cause collateral damage to surrounding cells. Similarly, a destructive shockwave, which may be used to rupture a cell membrane in order to lyse the cell (e.g., as in cancer treatments) may also impair or destroy nearby healthy tissue. To address this problem, we use dissipative particle dynamic (DPD) simulation to investigate the addition of a cavitation bubble between the shockwave and the model cell membrane to alter the shockwave front, allowing low-velocity shockwaves to specifically damage an intended target. We focus specifically on a spherical lipid bilayer model, and note the effect of shockwave velocity, bubble size, and orientation on the damage to the model cell. We show that a cavitation bubble greatly decreases the necessary shockwave velocity required to damage the lipid bilayer and rupture the model cell. The cavitation bubble focuses the kinetic energy of the shockwave front into a smaller area, inducing penetration at the edge of the model cell. With this work, we provide a comprehensive approach to the intricacies of model cell destruction via shockwave impact, and hope to offer a guideline for initiating targeted cellular destruction using induced cavitation bubbles and low-velocity shockwaves.

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Title: Strain Field Approximation and Crack Tracking using the Particle Difference Approximation

Author(s): *Andrew Beel, Jeong-Hoon Song, *University of Colorado Boulder*; Athanasios Iliopoulos, John Michopoulos, *U.S. Naval Research Laboratory*.

From a modeling and simulation perspective, detection and accurate quantification of crack trajectories from full field measurement tests is vital to validating models of crack initiation, propagation, and branching. From an application domain perspective, detection and quantification of crack trajectories is essential for structural health monitoring applications. This study examines how the Particle Difference Approximation (PDA) [1-2], a meshfree point collocation method, can be applied to approximate strain fields that can subsequently be used to detect the trajectory of a crack in a material test sample. The PDA allows for numerical computation of differential operators based on a Taylor polynomial expansion of the displacement fields. Using the differential operators afforded by the PDA, the strain and surface strain compatibility functional (SSCF) [3] can be computed directly from the measured displacement fields in a material test by many full field measurement methods. Calculating derivatives of the displacement fields using the PDA was found to be accurate and computationally efficient. These advantages of the PDA, coupled with the SSCF method for detecting the crack trajectory, result in accurate and efficient calculation of strain and crack trajectory tracking in a structural component regardless of the loading and the mechanical properties of the material. This presentation will discuss the efficacy of the PDA to represent strain fields directly and to detect the trajectory of a crack in a 2D sample subjected to a numerical (synthetic) experiment and compare these results to those from the existing mesh-free strain representation method [3]. References: [1] Y.C. Yoon and J.H. Song, “Extended particle difference method for weak and strong discontinuity problems: Part I. Derivation of the extended particle derivative approximation for the representation of weak and strong discontinuities”, Computational Mechanics, 53:1087-1103 (2014). [2] Y.C. Yoon and J.H. Song, “Extended particle difference method for weak and strong discontinuity problems: Part II. Formulations and applications for various interfacial singularity problems”, Computational Mechanics, 53:1105-1128 (2014). [3] A. Iliopoulos and J.G. Michopoulos, “On the feasibility of crack propagation tracking and full field strain imaging via a strain compatibility functional and the Direct Strain Imaging method”, International Journal of Impact Engineering, 87:186-197 (2016).

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Title: Higher-Order Elements for Explicit Solid Dynamics

Author(s): *Stephen Beissel, Timothy Holmquist, *Southwest Research Institute*.

Higher-order finite elements have gained widespread use in computational hydrodynamics due to performance superior to that of first-order elements. In contrast, first-order elements are still used almost exclusively in commercial software for explicit solid dynamics. One likely reason for this exclusion is the primary importance historically placed on minimizing the number of floating-point operations required for the evaluation of the internal-force term in the equations of motion, since these evaluations consume the majority of CPU time of explicit analyses. In this presentation, a formulation of higher-order finite elements for explicit solid dynamics is introduced, and the performances of various element orders are compared to that of widely used first-order elements. The elastic response of a simple part loaded by a single pulse is quickly transformed into complex high-frequency waves by reflections at the part boundaries. Computations of this transformation demonstrate the ability of higher-order elements to resolve high-frequency waves much more accurately than first-order elements when errors are plotted as a function of mesh refinement. Since the number of floating-point operations required for the evaluation of the internal forces increases with the element order, errors are also plotted as a function of computing (wall-clock) time. From this perspective, the computational effort required to attain a desired degree of accuracy is much less with higher-order elements. When the errors are plotted as a function of allocated memory, the higher-order elements are also shown to require much less memory to attain a desired degree of accuracy. Some additional considerations for the successful implementation of higher-order elements in general-purpose explicit codes are addressed in less detail than wave propagation. In particular, computations involving plastic deformations indicate that the higher-order elements do not appear to suffer from the locking phenomenon that plagues fully integrated first-order elements.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: From Full-Field Measurements to Material Properties of Composite Materials

Author(s): *Cedric Bellis, Manel Trabelsi, *LMA CNRS*; Flavien Fremy, *Saint-Gobain, Northboro R&D Center*.

This presentation focuses on imaging and characterization for composite materials. These are understood in the broad sense of materials that are composed of multiple constituents with different properties or functionalities. The overarching goal in this area is to be able to reconstruct quantitatively a constitutive material parameter distribution of interest that characterizes an investigated body or sample. To achieve that objective new insights have been gained over the last twenty years with the flourishing and success of full-field measurement techniques in many areas of physics such as those based on digital image correlation, X-ray or neutron diffraction tomography, ultrasound or magnetic resonance. Overall, these experimental methods permit to monitor the response of a given medium under an applied external loading so as to obtain internal measurements that can be related to physical fields such as displacement, temperature or electric potentials to name but a few examples. In this context the typical available data is a set of digital images, which is nonetheless seldom handled as such when solving the inverse problem. In the context considered, the originality of the proposed method is to adopt the viewpoint of an image processing technique, using in particular a deconvolution algorithm implemented in the Fourier domain. This method permits to reconstruct the targeted constitutive material parameters by a direct analysis of the available full-field measurements that correspond to the set of experimental displacements, temperature or electric “images”. The proposed method is built on an iterative gradient-based algorithm and the fast Fourier transform for optimal performances. The proposed method permits to reconstruct quantitatively unknown material parameters by a direct deconvolution of a given set of full-field measurement “images”. Its principal features are as follow: 1) Meshless method that uses pixelized (2D) or voxelized (3D) images. 2) Fast and highly parallelizable due to intensive use of fast Fourier transforms (potential for live identification). 3) Multiple experiments can be combined to enhance the reconstruction quality. 4) Noise affecting the measurements is efficiently handled in Fourier space (regularization). 5) A variety of material configurations can be handled: conductivity or elasticity models, isotropic or anisotropic material configurations, etc. 6) Amenable to real-time identification of materials based on GPU implementation, therefore potential for online characterization or quality control. The performance of the method will be demonstrated on a set of numerical examples.

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Title: Experimental and Numerical Investigation of the Turbulent Flow over D-Shaped Bluff Body

Author(s): *Alla Eddine Benchikh Lehocine1, Jay Lacey, Sébastien Poncet, *Université de Sherbrooke*.

Many numerical and experimental studies have been performed to investigate turbulent flows around obstacles, however only a few of them focus on bed mounted obstacles. In the present work, open-channel flow over a D-shaped bluff body were studied by planar and stereoscopic particle image velocimetry (PIV). A numerical benchmark of different turbulence closure models was also performed. The SST low-Re model was found to be more adapted at representing the shear layer while the k-ω and k-ω SST models demonstrated higher accuracies in the recirculation region. Large eddy simulations (LES) were performed over the D-section to determine the influence of the sub-grid scale models on the prediction of the vortical structures. The WALE model showed a better overall agreement, contrary to the Smagorinsky model, which was too dissipative. Various discretization schemes were also evaluated highlighting the superiority of a central second-order difference scheme chosen for its lower dissipation. Keywords—Bluff Body, Stereoscopic PIV, Turbulence models, Large Eddy Simulation.

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Title: On the Solution of Free Surface Problems by Lagrangian and Semi-Lagrangian Galerkin Methods

Author(s): *Marta Benítez, *University of A Coruña*; Alfredo Bermúdez, *University of Santiago de Compostela*; Pedro Fontán, *Technological Institute for Industrial Mathematics (Santiago de Compostela)*.

In the present work we present new Lagrangian and semi-Lagrangian methods for solving free surface problems. Specifically, fluid-dynamics problems in a time dependent domain and fluid-structure interaction problems are considered. The governing equations for the fluid are the unsteady incompressible Navier-Stokes equations. Typically, they are based on a Eulerian formulation in terms of the velocity in contrast to the usual Lagrangian formulation in terms of the displacement for the solid equations. Therefore, a typical difficulty for solving fluid-structure interaction problems is coupling at the interphase. Moreover, in fluid-dynamics problems with free surface flows, the Eulerian formulation of Navier-Stokes equations presents two classical difficulties: the treatment of the convective term and the modelling and tracking of the free surface. These problems have been solved with several Lagrangian approaches (see, for instance, [3]). In the present work Lagrangian and semi-Lagrangian approaches are used (see [1] and [2] for details). A quite general change of variable from the current configuration to a reference configuration, not necessarily the one of the initial time, is proposed obtaining a new formulation of the problem, in terms of the displacement or velocity, from which classical and new time discretization methods can be introduced in a natural way. Different second-order temporal integration schemes based on Newmark schemes are considered. We notice that the second-order and unconditionally stable Newmark scheme leads to solve at each time step a non-linear problem. However, most methods that we propose are linear. These temporal integration schemes are combined with finite element approximations for the numerical solution of the problems. In order to assess the performance of the proposed numerical methods, we solve different free surface problems in two space dimensions. [1] M. Benítez and A. Bermúdez, Second-order pure Lagrange-Galerkin methods for fluid-structure interaction problems, SIAM J. Sci. Comput., 37:B744-B777, 2015. [2] M. Benítez and A. Bermúdez, Pure Lagrangian and semi-Lagrangian finite element methods for the numerical solution of Navier-Stokes equations, Appl. Numer. Math., 95:62–81, 2015. [3] S. Idelsohn, E. O˜nate and F. Del Pin, The particle finite element method: a powerful tool to solve incompressible flows with free-surfaces and breaking waves, Int. J. Numer. Meth. Eng., 61:964-989, 2004.

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Title: Network Model of Re-Entrant and Conventional Cellular Materials

Author(s): *Igor Berinskii, *Tel Aviv University*.

A relatively simple two-parametric model is proposed to perform a qualitative analysis of cellular materials. The model describes microstructure as a network of axial and torsional linear springs. A discrete-to-continuum procedure is proposed to determine the effective properties of solid material corresponding to the re-entrant and regular honeycombs. The procedure is based on comparison of strain energies of the structures and corresponding orthotropic material. The components of stiffness tensor and Poisson's ratio of the structures were studied as a function of interaction parameters and the angles between the structural elements. It was shown that re-entrant honeycombs always demonstrate the auxetic properties, whereas the isotropic regular honeycombs can have negative Poisson's ratio at some combination of longitudinal and torsional stiffness between the nodes. A model was calibrated to real materials and structures to demonstrate its usability for simulations.

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Title: A Minus One Norm Stabilized DG Method on Polygonal Meshes

Author(s): *Silvia Bertoluzza, Daniele Prada, *CNR, IMATI "Enrico Magenes"*.

The stability of DG methods relies, among other things, on the action of stabilization terms which penalize some residual, usually in a mesh dependent norm designed to mimic the norm (which is usually quite cumbersome to evaluate) of the dual space where the residual naturally exists. Estimates on the resulting methods are depending on the existence of direct and/or inverse inequalities relating the mesh dependent norm to the natural dual norm it is designed to mimic. In this talk we discuss the possibility of directly designing computable dual norms and of using them as stabilization term in a DG type method. Based on this idea we propose a DG method for solving the Poisson equation on polygonal meshes, in which the unknown in the polygonal elements, the fluxes, and the unknown on the edges, are all, independently, approximated by polynomials of degree k. Well posedness is achieved using a suitable “minus one norm” stabilization term penalizing the discrepancy between actual the fluxes of the discrete solution in the elements, and the unknown that independently discretizes the fluxes. A theoretical analysis of the method will be presented, together with numerical tests.

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Title: Reliable Large Scale Industrial Design at Petascale and Beyond

Author(s): *Martin Berzins, *University of Utah*.

The moves to petascale and exascale computers have made possible to engage in the industrial design simulations of scales that are significantly larger than what has been possible until now. An outstanding example of such simulations using the Uintah software will be described. The example is that of a 20,000 cu M coal boiler currently deployed by GE/Alstom. The Uintah software will be described and its application to this problem considered. In order to solve a problem at this scale a number of changes had to be made in a number of key areas of the code. Scalability results up to about 500K cores on DOEs Mira computer will be shown. The challenges of addressing thermal heat transfer using radiation will be considered and a ray tracing approach employed. The results of simulations using a 450M cpu hours allocation via the INCITE program will be shown. The challenge of going to future architectures such as Aurora and beyond to exascale will be described.

14th U.S. National Congress on Computational Mechanics
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Title: Countering the Curse of Dimensionality in Data-Driven Design of Materials and Structures

Author(s): *Miguel A. Bessa, Sergio Pellegrino, *Caltech*; Wing kam Liu, *Northwestern University*.

Data-driven computational design of materials and structures usually requires the construction of large databases containing the predicted response of different designs under specified loading conditions. This data-driven approach to design is usually limited by the substantial computational expense of building large databases, especially when modeling irreversible processes such as plasticity and damage. A new data-driven computational framework integrating the recently developed self-consistent clustering analysis method is shown to address this longstanding challenge for the first time, opening avenues to the discovery of innovative materials with new capabilities in an era of high-throughput computing (“big-data”).

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Title: Towards the Identification of Damage Parameters from Full-Field Measurements within the Finite Strain Framework

Author(s): *Francesco Bettonte, Sylvia Feld-Payet, David Lévêque, *ONERA The French Aerospace Lab*; Jacques Besson, *Mines ParisTech, Centre des Matériaux*.

Numerical simulation is used in designing and prototyping to reduce the number of mechanical tests or to dimension structures for which a real-size test is not conceivable. Reliability of these numerical simulations largely depends on the underlying model parameters, and thus on their identification. The objective of this contribution is to propose a robust strategy for the identification of damage parameters based on a small number of mechanical tensile tests. Tests are carried out on flat and axi-symmetric notched specimens, which are observed with a stereo vision system. A Digital Image Correlation software developed at Onera provides surface full-field measurements. These outputs are used to perform parameter identification via a Finite Element Model Updating (FEMU) technique, which is based on the comparison between experimental full-field measurements and their simulated counterparts. In order to ensure the comparison's validity, the measured displacements are prescribed as boundary conditions to the simulation. This also implies that the measurement noise could potentially be prescribed with unpredictable effects. To overcome this problem a noise filtering technique is used. The described identification strategy is applied to a nickel-based superalloy undergoing large deformations. The logarithmic approach proposed by Miehe-Apel-Lambrecht coupled with a GTN damage model is employed. The main challenge regards the modelling of the softening behaviour. When standard damage models are used, strain (and consequently damage) spuriously localizes within a finite band of elements. To overcome this problem a mixed non-local extension of the Miehe-Apel-Lambrecht element is used. The internal length introduced by the non local formulation acts as regularization parameter and can be seen as an additional information about the internal structure of the material. It is directly related to the effective size of the strain localization band. The identification of this additional parameter via FEMU is investigated. Finally, in order to validate the proposed strategy, the identified parameters are used to simulate a tensile test on a complex 3D geometry (inspired by the first Sandia Challenge). The dissipated energy and the size of the strain localization band are used as criteria to evaluate the identification strategy.

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Title: Nondestructive Measurement of Thermal Diffusivity of Bodies of Arbitrary Shape

Author(s): Wojciech Adamczyk, *Ryszard Bialecki, Tadeusz Kruczek, Ziemowit Ostrowski, *Silesian Univ. Technology*.

Heat diffusivity is retrieved by solving an inverse heat transfer problem in samples of arbitrary shape whose geometry is grabbed by a laser scanner. Temperature field is induced by a laser flash impinging directly on the surface whose temperature is recorded by an IR camera. Levenberg Marquardt technique yields then the components of the anisotropic heat diffusivity tensor. The method has been applied to retrieve the heat diffusivity of both the substrate and a thin layer coating. Various techniques of solving the direct problem in the sample are discussed: analytical solution of the semi-infinite medium problem, numerical solution of the heat conduction equation in the sample, numerical model taking into account the CFD solution of the air in contact with the sample. To speed up the evaluation of the direct problem, a reduced order method has been used. The solution has been expressed as a linear combination of Proper Orthogonal Decomposition modes whose amplitudes were approximated using Radial Basis Function to account for the dependence on time and components of the diffusivity tensor. The results were compared with the measurements using a commercial laser flash apparatus based on the Parker's method. Good accuracy of the proposed technique has been obtained. An apparatus based on the developed technique is embedded into a carbon lining and electrodes production line, where the on-line measurements are used to quality control of the manufactured materials. The solution is protected by a pending patent. Acknowledgements This research has been supported by the National Science Center within the OPUS scheme, under contract UMO-2013/11/B/ST8/00268 and the SONATA scheme under contract\\ UMO-2014 /15/D/ST8/02620. References [1] W. Adamczyk, Z. Ostrowski, Retrieving thermal conductivity of the solid sample using reduced order model inverse approach, International Journal of Numerical Methods for Heat and Fluid Flow, 2016, acccepted DOI (10.1108/HFF-05-2016-0206) [2] W. Adamczyk, R. Bialecki, T. Kruczek, Patent application,EP11195498.8 (December 23, 2011)

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Title: Bayesian Selection of Optimal Physics-Based Model and Modeling Error

Author(s): *Philippe Bisaillon, Rimple Sandhu, Abhijit Sarkar, *Carleton university*; Mohammad Khalil, *Sandia National Laboratories*; Chris Pettit, *United States Naval Academy*; Dominique Poirel, *Royal Military College of Canada*.

Numerical models in engineering are imperfect, thereby leading to errors in the predictions that can not be accounted by just measurement errors. These errors occur due to the inherent simplification and approximations in the mathematical modeling of a complex physical phenomenon. To improve the efficacy of a model, the first approach is to better capture the missing physical aspects of the phenomenon at hand. Whenever the first approach is no longer feasible (for instance, due to computational bottlenecks). the second approach involves adopting complex modeling errors. For stochastic ordinary differential equations, the modeling error is often modeled as a Gaussian white noise for simplicity. A more complex modeling error may compensate the effects of unmodelled physics and improve the predictive capabilities of the models. In this work, the authors investigate the usefulness of the Gaussian colored modeling noise (error) in nonlinear dynamical systems. To demonstrate the benefit of colored noise for modeling error, a nonlinear aeroelastic system undergoing limit cycle oscillations is simulated using unsteady aerodynamic loading. A candidate set of quasi-steady aerodynamics models (having increasing complexities) with both white and colored modeling errors are proposed. Using a Bayesian framework for parameter estimation and model selection, the optimal quasi-steady aerodynamic model and optimal error model are selected. The effects of the sparsity of the observational data and model complexity are also investigated.

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Title: Reciprocal Mass Matrices in Explicit Dynamics – Inertia Scaling and Customization

Author(s): Anne-Kathrin Schäuble, Anton Tkachuk, *Manfred Bischoff, *University of Stuttgart*.

In recent years, selective mass scaling techniques became a popular means to increase the critical time step in explicit dynamics. The resulting non-diagonal mass matrices, however, compromise computational inefficiency, as computation of the accelerations requires the solution of a linear system of equations at every time step. Still, the diagonal (lumped) mass is most often used in explicit dynamics, even though its usage may deteriorate accuracy, especially for higher order, tetrahedral and isogeometric finite elements. A novel approach allows the direct construction of sparse inverse mass matrices, thus circumventing the aforementioned equation solving while retaining some of the beneficial properties of selective mass scaling. It is based on a three-field, parametrized Hamilton's principle with independent shape functions for displacement, velocity and linear momentum. The current contribution presents an extension of this method, using a mass-specific linear momentum field, which allows for mass preservation in case of non-constant density. Introducing a free parameter template in the parametrized Hamilton's principle provides control over different ansatz spaces. It does not only allow for tuning the method for speed-up (inertia scaling) but also for higher accuracy (inertia customization). Application of this approach to transient analyses is presented with focus on isogeometric finite elements. Furthermore, applications to contact problems and efficient time step estimators are discussed.

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Title: Polyhedral Discretizations Using Tetrahedral Subdivisions for Applications in Nonlinear Solid Mechanics

Author(s): *Joseph Bishop, *Sandia National Laboratories*; N. Sukumar, *University of California, Davis*.

For geometrically complex parts and systems, the time required to develop an analysis capable finite element mesh can still take days to months to develop, despite vast increases in computing power. Advanced tetrahedral meshing tools can alleviate this burden, but the development of robust and efficient tetrahedral finite-element formulations for applications in large-deformation solid-mechanics is still an active area of research. The recent development of general polyhedral formulations for solid mechanics offers an opportunity to ease this meshing burden. Starting with an existing tetrahedral mesh, we first subdivide each tetrahedron using standard rectification techniques. Two types of polyhedra are formed from the tetrahedral subdivisions: (1) an aggregation of subtetrahedra attached to the original nodes, and (2) either an octahedron with 6 vertices or a polyhedron with 12 vertices and 8 faces, depending on the degree of rectification. Several approaches may then be used to define the shape functions (e.g. using harmonic or maximum entropy coordinates) and quadrature schemes for the new polyhedra in order to obtain a consistent and stable finite element formulation. Verification problems and examples are presented.

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Title: Modeling of Solidification and Thawing Problems with Free Surfaces in Rigid Containers

Author(s): *Bruno Blais, *National Research Council* ; Florin Ilinca, *National Research Council*.

The modelling of freezing and thawing process is a challenging topic which has recently garnered increasing industrial interest. An example lies in the storage of AdBlue, a urea-water solution which is used for the Selective Catalytic Reduction (SCR) of the exhaust gas of diesel engines [1]. The implementation of this technology, which has the potential to greatly reduce nitrogen oxides (NOx) emissions, faces considerable challenges in colder regions of the world since AdBlue freezes and expands around -11°C. This can put considerable stresses on the containers storing the fluid. Thus, it is important to develop robust numerical models that can simulate freezing and thawing in such configurations in order to ensure adequate design and operations of SCR components. The modelling of phase change is complex since it includes sharp moving interfaces, an issue that may be exacerbated by the occurrence of natural convection. Since the latter has a considerable influence on the position of the thawing or freezing front, models become inherently complex due to the coupling between the solid-liquid discontinuity, the natural convection, the non-linear variations of the physical properties of the material (such as the density, specific heat or viscosity) and the multiple time scales at which these interactions take place. In this work, we present a novel implicit finite element model for phase changes with natural convection that takes into account the deforming free surface between the liquid and air as well as the thermal expansion of the liquid as it undergoes phase change. The model uses a classical Eulerian formulation to describe the liquid and solid phases while keeping track of the fluid-air interface using a Level Set approach. This allows for the simulation of phase changes on a static Eulerian mesh without requiring a specific treatment of the solid-fluid interface, while maintaining the capacity to simulate the thermal expansion due to the phase change, thus enabling simulation of three co-existing phases. The model is verified, then validated on realistic test cases and compared to experiments. Finally, an extension of the model to take into account fluid-structure interaction due to the expanding solid is discussed. [1] aus der Wiesche, S. (2007). Numerical heat transfer and thermal engineering of AdBlue (SCR) tanks for combustion engine emission reduction. Applied thermal engineering, 27(11), 1790-1798.

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Title: Thermally-Driven Oscillatory Cracks and Branching Cracks in Glass: A Peridynamic Analysis

Author(s): *Florin Bobaru, Zhanping Xu, Guanfeng Zhang, *University of Nebraska-Lincoln*.

Oscillatory and surprisingly stable crack growth in glass has been observed experimentally in thermally-driven fracture of thin glass plates. This behavior is obtained by slowly immersing a hot thin glass plate with a small pre-notch in a bath of cold water. Depending on several parameters (immersion speed, width of plate, temperature gap between the oven and the cold bath) one observes one of the following: no crack growth, growth of a straight crack, an oscillatory crack, or a crack that branches and branches may show oscillations. It has also been observed that the wave-length of the oscillatory crack depends on the plate width and immersion speed. While a variety of computational modeling approaches have been used in the recent past to try to predict this complex behavior, none so far have been able to capture the entire spectrum of observed crack types. We present a peridynamic model for thermomechanical failure and use it to test its ability of reproducing the fracture phase-diagram of the above-mentioned experiments. We use quasi-static solver and, for convenience, import the temperature field measured experimentally. We show that a conventional failure criterion used in peridynamics requires a certain enhancement for this type of small-deformation problems. With the new criterion, the peridynamic model matches the experimentally observed behavior over the slow immersion speed regime, including the nonlinear curves that separate different crack types in the fracture phase-diagram of immersion speed and plate width. The model correctly predicts the location of the crack tip, in time, to be near the oven, and closer to the oven with higher immersion speed. We explain the possible reasons for why phase-field or XFEM models of this problem, for example, have not been able to predict the complexity of crack growth behavior in thermally-driven fracture. The results show that a simple model (linear thermoelastic peridynamic model) is sufficient to explain the behavior observed experimentally. References: [1] Zhanping Xu, Guanfeng Zhang, and Florin Bobaru. Predictability of thermally-driven cracks in glass. (submitted) 2017.

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Title: Anisotropic A Posteriori Error Estimation and Mesh Adaptation for the Monodomain Model in Cardiac Electrophysiology

Author(s): *Edward Boey, Yves Bourgault, Thierry Giordano, *University of Ottawa*.

This talk concerns error estimation and adaptive methods for the nonlinear monodomain system used for simulation of the action potential in cardiac electrophysiology. The system consists of a parabolic PDE representing the transmembrane potential, coupled with a system of first order ODEs for the ionic/gating variables. Numerically, these problems tend to be stiff, and can be demanding in terms of computational resources. In particular, the solutions tend to develop sharp wave fronts, and for certain ionic models exhibit multiscale behaviour. Achieving accurate solutions with uniform spatial and temporal resolutions can often be impractical. Anisotropic residual error estimates for elliptic equations were introduced by Picasso [1] based on interpolation estimates by Formaggia and Perotto [2]. Mesh adaptation is performed with the aid of a non-Euclidean metric derived from the estimator. In this way, one controls the error not only with the size of the elements, but with the alignment of the elements with respect to the metric. The primary contribution presented in this talk is the extension of their estimator and adaptive methods to the monodomain system. The ionic variables do not benefit from the smoothing properties of a diffusion operator, giving rise to numerical difficulties in the adaptive algorithm. In addition, the mesh adaptation will be coupled with adaptive time stepping for the BDF2 method using a new error estimator. The BDF2 estimator extends results for linear ODEs by Akrivis and Chatzipantelidis [3] to nonlinear parabolic PDEs. The talk will include numerical examples and a discussion on the efficiency of the method for various ionic models, both continuous and discontinuous. References: [1] M. Picasso, An anisotropic error indicator based on Zienkiewicz-Zhu error estimator: application to elliptic and parabolic problems, SIAM J. Sci. Comput. 24(4) 4, p. 1328-1355 (2003) [2] L. Formaggia and S. Perotto, New anisotropic a priori error estimates, Numer. Math. 89, p. 641-667 (2001). [3] G. Akrivis and P. Chatzipantelidis, A posteriori error estimates for the two-step backward differentiation formula method for parabolic equations, SIAM J. Numer. Anal. 89(1), p. 109-132 (2010).

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Title: A Posteriori Finite Element Methods for Mixed Eigenvalue Problems

Author(s): *Daniele Boffi, *University of Pavia*.

In this talk I review the design and the analysis of adaptive finite element schemes for the approximation of eigenvalue problem arising from partial differential equations. Starting for basic examples, I discuss the case when multiple eigenvalues or clusters of eigenvalues are present. The main application is the approximation of the eigenvalues of the Maxwell cavity problem.

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Title: Discontinuous Galerkin Methods for Maxwell's Equations in Nonlinear Polarization Media

Author(s): *Vrushali Bokil, *Oregon State University*; Yingda Cheng, Yan Jiang, *Michigan State University*; Fengyan Li, *Rensselaer Polytechnic Institute*.

The propagation of electromagnetic waves in a material is modeled by the time-dependent Maxwell's equations along with constitutive laws that describe the response of the medium to the electromagnetic field. Recent optics and photonics research has focused on phenomenon at smaller and smaller length scales or multiple scales so that the full-wave time domain Maxwell equation based models and nonlinear imaging techniques have become necessary to adequately capture useful optical effects and solve current nonlinear optics problems. In this talk, we consider a nonlinear dispersive model comprising of Maxwell's equations along with a system of nonlinear ordinary differential equations, where the nonlinearity comes from the instantaneous electronic Kerr response and the residual Raman molecular vibrational response, together with the single resonance linear Lorentz dispersion. The modeling approach is referred to as the Auxiliary Differential Equation (ADE) approach in the computational electro-magnetics literature. To design efficient, accurate, and stable computational methods for this nonlinear Maxwell model, we apply high order discontinuous Galerkin discretizations in space. We prove that the resulting semi-discrete methods are stable. The challenge to achieve provable stability for fully-discrete methods lies in the temporal discretizations of the nonlinear terms. To overcome this, novel modifications are proposed for both the second-order leap-frog and implicit trapezoidal temporal schemes. The performance of the proposed methods are further demonstrated through numerical experiments. We study the decay of higher-order solitons under the combined action of dispersion, self-phase modulation, self-steepening, and stimulated Raman scattering, and the development of a kink and anti-kink wave solution that develops due to the Kerr nonlinearity.

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Title: Nondeterministic Parameter Calibration for Crystal Plasticity Models

Author(s): *Geoffrey Bomarito, Patrick Leser, James Warner, Jacob Hochhalter, *NASA*; Timothy Ruggles, Saikumar Yeratapally, *NIA*.

Phenomenological parameters used in crystal plasticity finite element models are calibrated by solving an inverse problem, typically by enforcing agreement between a computed and measured force-displacement curve. Although this provides an homogenized equivalence of the macroscopic be- havior between model and experiment, it precludes the understanding of any inherent variability in the model parameters. Nonetheless, from more fundamental analysis it is expected that such parameters will have both random and systematic variations throughout the microstructure. For ex- ample, resistance to slip may vary systematically, depending on proximity to grain boundaries or second phases, and randomly, due to variations in the strength and density of precipitates. While much effort is being fo- cused on capturing the effect of microstructure morphology distributions on material behavior, relatively little focus is placed on acquiring anal- ogous distributions of the underlying constitutive model parameters. In this work, full-field strains are obtained using digital image correlation and the inverse problem is constructed based on point-wise data through- out the domain, as opposed to a single homogenized result. In an initial step, simplifying Taylor approximations are made to obtain distributions of the constitutive parameter estimates. This initial step serves to nar- rowly bound the parameter distributions. After reducing the parameter domain space, an inverse finite element method is used to compute spatial correlations among the parameters and microstructural features. Consid- eration of nondeterministic constitutive model parameters will enhance the representation of stochastic material behavior within the finite ele- ment method. Furthermore, this approach will interface more naturally with lower length scale models, where events underpinning material be- havior are represented as probabilities.

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Title: Reduced-Order Compensators for Estimation and Feedback Flow Control

Author(s): *Jeff Borggaard, *Virginia Tech*.

Development of reduced-order models (ROMs) for the feedback control of fluids is critical and remains an active area of research. The main advantage of ROMs in designing feedback controllers is the reduced-dimension of the model that enables the design of the feedback law. However, in any practical problem, limited measurements necessitates the creation of state estimators, or compensators, that can be simulated fast enough for real-time implementation yet produce control inputs that maintain an acceptable level of performance (and at least stability) in closed-loop simulations. While it may seem natural to reuse the ROM for the control design to compute the compensator, the requirements for the ROM are very different. However, the ROM for the compensator cannot be built in isolation as it must estimate the "controlled" system. We present an overview of several strategies for compensator design, including the attractive, though often unfeasible, "design-then-reduce" approach. While unfeasible, it does offer motivation for the understanding and development of more practical algorithms. We study a number of these issues using a model feedback flow control problem, stabilizing the wake behind a pair of cylinders. For the feedback design, we apply interpolatory model reduction (interpolation of the input-output transfer function) on the Oseen equations. For the compensator design, we ultimately build a nonlinear model to estimate the state from a few velocity measurements. We explore several options for this, including the proper orthogonal decomposition (POD), goal-oriented variants, and modifications of the interpolatory model reduction strategy.

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Title: A High-Order Discontinuous Galerkin Method for Variable-Coefficient Advection-Diffusion Problems

Author(s): *Raunak Borker, Charbel Farhat, Radek Tezaur, *Stanford University*.

A high-order Discontinuous Galerkin Method with Lagrange Multipliers (DGLM) is presented for the solution of the steady advection-diffusion equation with a variable advection field in the high Peclet number regime. In this regime, the standard Finite Element Method (FEM) typically produces non-physical oscillations at practical mesh resolutions. Like a Discontinuous Enrichment Method (DEM) [1], the DGLM method described in this talk overcomes the issue of spurious oscillations near boundary layers by attempting to resolve them using enrichment shape functions. Here, these non-conforming functions are chosen as discontinuous polynomials that are additively enriched with free-space solutions of an approximation of the governing differential equation obtained using asymptotic analysis. This approximation leads to enrichment functions for both exponential and parabolic boundary layers. Also like a DEM, the DGLM method presented here enforces a weak continuity of the solution approximation across inter-element boundaries using carefully chosen Lagrange multiplier fields, and is amenable to an efficient implementation using static condensation. It is proven to be well-posed, and to require no stabilization. Its superior performance is demonstrated for several model but representative problems in the high Peclet number regime. Its extension to unsteady problems can be performed using the framework presented in [2].
References: [1] C. Farhat, I. Harari, L. P. Franca, The discontinuous enrichment method, Comput. Methods Appl. Mech. Eng., 190, 6455- 6479, 2001. [2] R. Borker, C. Farhat, R. Tezaur, A high-order discontinuous Galerkin method for unsteady advection-diffusion problems, J. Comput. Phys., 332, 2017.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Modeling Model-Form Uncertainties in Eigenvalue Computations Using a Data-Driven Stochastic Reduced-Order Model

Author(s): Charbel Farhat, *Adrien Bos, Phil Avery, *Stanford University*; Christian Soize, *Université Paris Est*.

A feasible, nonparametric, probabilistic approach for quantifying model-form uncertainties associated with a computational model designed for the solution of a generalized eigenvalue problem is presented. It is based on the construction of a Stochastic, Projection-based, Reduced-Order Model (SPROM) [1] associated with a High-Dimensional Model (HDM) using three innovative ideas: the substitution of the deterministic Reduced-Order Basis (ROB) with a stochastic counterpart (SROB) featuring a reduced number of hyperparameters; the construction of this SROB on a subset of a compact Stiefel manifold in order to guarantee the linear independence of its column vectors and the satisfaction of the boundary conditions; and the formulation and solution of a reduced-order inverse statistical problem to determine the hyperparameters so that the mean value and statistical fluctuations of the eigenvalues predicted using the SPROM match target values obtained from available data. Consequently, the proposed approach for modeling model-form uncertainties can be interpreted as an effective approach for extracting fundamental information or knowledge from data that is not captured by a deterministic computational model, and incorporating it in this model. Its potential for quantifying model-form uncertainties in eigenvalue computations is demonstrated for sample natural vibration analysis problems associated with aircraft structural engineering. [1] C. Soize and C. Farhat, "A Nonparametric Probabilistic Approach for Quantifying Uncertainties in Low- and High-Dimensional Nonlinear Models," International Journal for Numerical Methods in Engineering, Vol. 109, pp. 837-88 (2017)

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Modeling Heterogeneities Effects on Phase Transformation during Quenching of Large Size Forged Steel Ingots

Author(s): *Yassine BOUISSA, Henri Champliaud, *École de technologie supérieure*; Mohammad Jahazi, *École de technologie supérieure* ; Louis-Philippe Lapierre-Boire, Jean-Benoit Morin, *Finkl Steel - Sorel*; Nicolas Poulain, *Transvalor Americas*.

Currently, industrial competition requires quench hardening on increasingly massive parts in order to obtain high mechanical properties even at the center of the forged ingots for applications such as plastic injection molds. These steels are produced by ingot casting followed by forging for hardening, shaping and removing solidification defects. To reach high mechanical properties the quench process is used at the final stage followed by tempering to reduce the magnitude of residual stresses induced by quenching [1]. The large size of the cast ingots induces significant thermal gradients during quenching which result in chemical heterogeneities (segregation), grain size changes, and different phases proportions from the surface to the center of the forged part [2]. In the present work, the quenching module of the FEM code FORGE® NxT software (Transvalor) was used to study the effect heterogeneities on phase transformation, especially the evolution of newly formed phases in order to simulate the quenching process of large size ingots. A combination of different chemical compositions and grain sizes were used as material inputs to design critical spatial configurations for heterogeneities in specific localized zones in the ingot. The mutual interactions between simulation variables were taken into consideration. The calculations of phase transformations' kinetics, properties of formed phases (pearlite, bainite, and martensite), temperature evolution in thermal field as well as the calculation of all types of induced strains and stresses were carried out. The temperature distributions predicted by the thermo-metallurgical FEM model was validated by instrumenting a medium size ingot. References: [1] Ahmet Kaynar, S.G., Mustafa Türkmen Investigation on the behaviour of medium carbon and vanadium microalloyed steels by hot forging test, M.A. Design, Editor. 2015. [2] A. Loucif, D.S., C. Zhang, M. Jahazi, L. P. Lapierre-Boire, R. Tremblay, Macrosegregation of Alloying Elements in Hot Top of Large Size High Strength Steel Ingot. Materials Science Forum, 2016. 879: p. 1176-1181.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: The Earth by TELEMAC

Author(s): *Sébastien E. Bourban, Michael S. Turnbull, Alan J. Cooper, *HR Wallingford, UK*.

Numerical modelling for environmental hydraulics studies, whether for research or consultancy, has historically focused on inland and coastal areas, mainly driven by the Saint-Venant equations in 1D or 2D. It has been financed over decades by human activities as water affects, is sourced and is somewhat tamed by growing populations. Consequently, advanced solvers have been developed to provide scientists and engineers with flexible unstructured meshes fitting manmade or natural waterlines, interaction of physical processes such as hydrodynamics, waves, or sediment processes, advanced mathematics with non-diffusive, monotonic and high-order numerical schemes, and parallelised domain decompositions to greatly speed up computation for ever more detailed simulations. With their extension to 3D for applications to stratified waters, these solvers have gradually allowed use of the Navier Stokes equations. Those industry-driven solvers that choose to open up their source codes have further benefited from research and development carried out by growing communities of users worldwide. The TELEMAC system (opentelemac.org) is one such suite of solvers. Contrarily, numerical modelling for the oceans has mainly been restricted to the research arena, and is mainly used to represent decades or centuries of evolution in the context of climate changes. While their global resolution and the complexity of their underlying density driven physical processes has increased with computer power to include coupling with atmospheric models, for instance, these developments have steered investments away from the underlying solvers. Ocean models remain few in number, based on regular grid and legacy codes, with perhaps simpler mathematics compared to their shallow water counterparts. With the rising costs of sourcing raw material such as oil, gas, bio-chemical compounds, human activities are gradually linking the shores to much deeper waters. It has, therefore, become essential for scientists and engineers to bridge the gap between environmental hydraulics and oceanography. Dr Sébastien E. Bourban of HR Wallingford, UK, will be presenting the conclusions of the first of three phases to bridge that gap, using the TELEMAC system to model the Earth. In this first phase, an unstructured mesh of the Earth at 1 km resolution is used to demonstrate TELEMAC's capability to propagate 10 of the most devastating tsunami waves or model the world's tides all under 1 hour with only half a dozen processors. Sébastien will take this opportunity to open up to international collaborations to complete the next two phases, modelling storms, surges and waves on the way to modelling the oceans.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Nonlinear and Random Vibrations of a Tensioned Cable Net

Author(s): *Reyolando Brasil, Marcia Helena Yamamoto Sato, *Federal University of ABC*.

We present a study on the nonlinear dynamics of a tensioned cable net roof. Both quasi-static loads, such as self-weight and initial pretension, and time varying random wind loads are considered. Step-by-step numerical time integration via Finite Differences is implemented to solve the nonlinear differential equations of motion. Mass and damping are considered lumped, and the elastic restoring forces are computed directly from the variation of length of the cables that are connected to each net node at each time step. Thus, the formulation is purely uses only inertia, damping and elastic forces vectors, no matrices being formed or inverted, leading to considerable less computational effort. As large displacements are considered, and large pretension axial forces are applied, geometric nonlinearity is present in the formulation. The random nature of wind forces is simulated using a synthetic wind approach. A large number of artificial load time histories are generated from the Canadian Wind Forces on Structures Code Power Spectrum Density Function. The resulting cloud of response maxima is statistically treated in a Monte Carlo type of analysis. Keywords: nonlinear dynamics; geometric nonlinearity; random vibrations; wind forces; finite differences.

14th U.S. National Congress on Computational Mechanics
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Title: Mesh Adaptation Based on a Hierarchical A Posteriori Error Estimator

Author(s): *Thomas Briffard, André Fortin, *GIREF, Université Laval*.

Anisotropic mesh adaptation has proved to be a powerful tool for the computation of very accurate approximations to the solution of a partial differential equation. The possibility of stretching the elements according to the variations of a solution contributes to the efficiency of the method. Adapted meshes often succeed in capturing very steep variations whereas regular meshes fail. In this talk, we will first describe a mesh adaptation algorithm first introduced in [1,2]. The method is based upon a hierarchical error estimator which can theoretically be applied to solutions of any degree. Moreover the procedure relies only on the approximation of the first order derivatives of the solution. This is an improvement compared to metric based adaptation methods which relies on the recovery of the Hessian of the solution, and thus on second order derivatives. We will illustrate the optimality of our approach on approximations of degree one and two, even on problems where the first order derivatives of the solution are singular. Even in these extreme cases, we shall see that optimal convergence rates can be reached. We will show that very anisotropic meshes can be obtain when needed. Examples will be exposed in both 2D and 3D. Examples with complex 3D geometries will also be addressed. Finally, we will consider mesh adaptation for time-dependent problems, with an application to a laminar flow around a cylinder. References: [1] R. Bois, M. Fortin, and A. Fortin. A fully optimal anisotropic mesh adaptation method based on a hierarchical error estimator. Computer Methods in Applied Mechanics and Engineering, 209-212:12–27, 2012. [2] A. Fortin, T. Briffard, and A. Garon. A more efficient anisotropic mesh adaptation for the computation of Lagrangian coherent structures. Journal of Computational Physics, 285(0):100–110, 2015.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Use of Finite Element Analysis to Model the Potential Damage Caused to Passenger Railcars by the Use of Explosives

Author(s): *Ian Bruce, Devon Wilson, *Arup*; Przemyslaw Rakoczy, *Transportation Technology Center, Inc*.

The mission of the U.S. Transportation Security Administration (TSA) is protection of the nation's transportation systems to ensure freedom of movement for people and commerce. In furtherance of its mission, TSA's Office of Security Technologies has contracted with Arup North America Ltd (Arup) and Transportation Technology Center, Inc. (TTCI) to conduct research to quantify the vulnerability of railcars and infrastructure to damage caused by the use of explosives. The main objectives of this ongoing research program is to develop tools to evaluate the performance of exiting railcar structures, develop potential mitigation measures for current railcars, and investigate advanced security systems for future designs under blast conditions. As part of this research work Arup has built detailed finite element (FE) models of a series of passenger railcars and investigated a number of different methodologies for applying blast loads to these models. The methodologies investigated include separate CFD analysis with the pressures mapped onto the FE model, an implementation of the ConWep equations, and a coupled fluid structure interaction (FSI) model. The results from these analyses have been compared with the results from full scale blast tests carried out by TTCI to determine the most appropriate blast loading methodology to be used for this type of analysis. This presentation summarizes the methodology, results and conclusions of Arup's and TTCI's investigation.

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Title: Global Sensitivity Analysis of a Selective Laser Melting Finite Element Model: Identification of Influential Parameters

Author(s): *Claire Bruna-Rosso, Ali gokhan Demir, Maurizio Vedani, Barbara Previtali, *Politecnico di Milano*.

Selective Laser Melting (SLM), as one of the additive manufacturing techniques which allow to 3D-print metal components has gained a lot of interest in the last years. Despite its growing popularity, this technology still suffers from a lack of process knowledge, standards and qualification, which are limiting factors for a wider industrial use. Numerical modeling is currently a standard tool in production engineering for process optimization and in some cases for a more comprehensive understanding of the process physics. However, inherent to any model implementation and computation are various sources of uncertainties and errors. It is of major importance to identify them and assess whether their influence on the model output is significant through a sensitivity analysis. That is why we propose here a Global Sensitivity Analysis (GSA) in order to determine which parameters are the most influential on the computational results variability. The model to be analyzed is an in-house nonlinear Finite Element Model (FEM) of the SLM process. It includes material properties thermal dependence, a dedicated algorithm to simulate both irreversible and reversible phase changes and an experimentally calibrated laser heat source. It was used in its 2D version for a single layer simulation to limit the computational load. The study was performed on 26 parameters including material properties, their dependence on temperature, laser related parameters, boundary conditions data, and other process parameters. The outputs retained are the computed maximal temperature and melt pool width and length. The sensitivity analysis was performed using the Elementary Effect (EE) method as recommended by Campolongo et al [1]. A total of 1485 simulations were performed. The analysis revealed that among the 26 input parameters, 11 of them do not have a significant effect nor on the outputs variability mean values $\mu*$ neither on their standard deviation σ. It showed that the most influential parameters are the laser power and the material power absorption. Process parameters affected mainly $\mu*$ while material related properties model affected mostly σ. The results put in evidence the parameters with higher priority in the modeling effort, sources of error to be considered also in a validation stage, and provide insight on which parameters should be prioritized for further studies, both experimental and computational. [1] Campolongo, F. et al. An effective screening design for sensitivity analysis of large models Environmental Modelling & Software, 2007, 22, 1509 - 1518

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Coupled Electrochemistry and Solid Mechanics of Li-ion Battery Electrodes

Author(s): *Victor Brunini, David Noble, Brad Trembacki, Mark Ferraro, Scott Roberts, *Sandia National Laboratories*.

Many of the active materials used in Li-ion battery electrodes undergo significant mechanical strain upon insertion and extraction of Li during the charge and discharge processes. These strains can cause significant stresses in the mesoscale structure of battery electrodes containing active particles, binder material, and electrolyte and can alter battery performance and capacity during the lifetime of the cell. There is growing interest in modeling this coupled multiphysics process on mesoscale structures obtained from experimental imaging techniques. In prior work we have demonstrated the ability to use the conformal decomposition finite element method (CDFEM) to generate meshes from experimental images and perform coupled electrochemistry and solid mechanics simulations on those meshes. However, since a contiguous, conformal mesh was used in that work the approach was unable to account for the effects of sliding and intermittent contact between particles. Here we present recent work using a code-code coupling approach involving multiple mesh definitions to enable modeling of sliding contact in these complex microstructures. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This is document SAND2017-1797 A

14th U.S. National Congress on Computational Mechanics
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Title: Probabilistic Outcomes Prediction in the ICU: Adding Uncertainty to APACHE

Author(s): *Corey Bryant, *Cerner Corporation*.

The introduction of the Acute Physiology, Age, and Chronic Health Evaluation (APACHE) system in 1981 was a ground breaking approach to evaluating and improving patient outcomes in the intensive care unit (ICU) [1]. It influenced decades of research in patient care in the ICU. Over time, improvement in medical treatments and new medications, as well as the proliferation of electronic medical records, has warranted recalibration, but the basic methodology has stood the test of time [2,3]. However, the mathematical models are rather simplistic, relying on the abundance of data captured in the ICU to drive predictive performance for key outcomes such as mortality and length of stay. The traditional modeling approach condenses the information provided from hundreds of thousands of ICU encounters to a single numerical prediction for each patient. In the present work, a more robust predictive model is developed by introducing uncertainty and relying on Bayesian techniques. Instead of a standard regression model, the parameters are treated as random variables, with distributions informed from deterministic calibration and historical data. The result is a probabilistic regression model that provides a predictive distribution of the outcome. From a clinical perspective, this can be seen as allowing for variability in the way factors affect outcomes across patients. A brief review of the APACHE methodology will be provided. Followed by a description of prior distributions and error (or discrepancy) model used. Finally, the calibration process and posterior distribution will be discussed. A comparison with the existing deterministic models will also be provided. References: [1] W. A. Knaus, J. E. Zimmerman , D. P. Wagner, E. A. Draper and D. E. Lawrence, "APACHE-acute physiology and chronic health evaluation: a physiologically based classification system," Critical Care Medicine, vol. 9, pp. 591-597, 1981. [2] W. A. Knaus, D. P. Wagner, E. A. Draper, J. E. Zimmerman, M. Bergner, P. G. Bastos , C. A. Sirio, D. J. Murphy, T. Lotring and A. Damiano, "The APACHE III prognostic system. Risk prediction of hospital mortality for critically ill hospitalized adults," Chest, vol. 100, no. 6, pp. 1619-1636, 1991. [3] J. E. Zimmerman, A. A. Kramer, D. S. McNair and F. M. Malila, "Acute Physiology and Chronic Health Evaluation (APACHE) IV: hospital mortality assessment for today's critically ill patients.," Crit Care Med, vol. 34, no. 5, pp. 1297-1310, 2006.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Adaptive Arlequin Method for Multiscale Brittle Fracture with Subgrid Length Scales

Author(s): *Eric Bryant, WaiChing Sun, *Columbia University*.

The Arlequin method enables concurrent couplings of subdomains of different length scales via handshake regions. Compatibility between the different subdomains is enforced by an energy functional, i.e. using Laplace multipliers, with the discrepancy of solution minimized across the subdomains. This method works well for cases where the region of interest can be predetermined. However, in many applications related to fracture and strain localization, the domain of interest may shrink or grow over time. The purpose of this research is to evolve the fine-scale domain based on the need to extract useful information locally. As an example, we model the brittle fracture problem using nonlocal variational eigen-fracture in the fine domain, while solving the elasticity problem in the coarse domain. As fracture propagates in the fine domain, the fine domain also extends accordingly such that the stress field behind and ahead of the crack tip can be properly resolved. The synthesis of the adaptive Arlequin method and the coupling between the nonlocal and local models across length scales, allows one to simulate subscale crack propagation in which the length scale is finer than the finite element size, and achieve Gamma convergence. Possible extensions to poromechanics and anisotropic brittle fractures are also discussed.

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Title: Long-Term Study of Bone-on-Chip to Monitor Stem Cell Derived Osteocyte Mechanotransduction

Author(s): *Elisa Budyn, *Ecole Normale Superieure de Cachan*; Samantha Sanders, *Ecole Normale Superieur ede Cachan*; Morad Bensidhoum, Herve Petite, *University Paris Diderot*; Eric Schmidt, *University of Illinois at Chicago*; Bertrand Cinquin, *Ecole Normale Superieure de cachan*; Patrick Tauc, *Ecole Normae Superieure de Cachan*.

With increasing life expectancy, pathologies related to massive bone loss carry $10 billion financial burden on the U.S. healthcare system. Successful techniques to repair massive tissue regeneration can be however difficult and require the addition of functional materials. We propose to build in vitro systems where human osteocyte progenitors are seeded in a previously decellularized human bone tissue for more than fifteen months. The systems are compared to in vitro systems seeded with mature osteocytes. To design successful cellularized implants it is essential to quantify the relationship between in situ mechanical stimulation and the cell biological response at different stages of their differentiation and to characterize the ECM formed by the seeded cells. Dual experimental and numerical top-down 3D investigations of bone-on-chip composed of progenitor and mature osteocytes reseeded on fresh human bones. These bones-on-chip showed the in vitro osteocyte biological response to in situ mechanical loads. The bone-on-chip were subjected to mechanical stimulation where controlled sub-microscopic damage near live osteocytes was produced. The local stress field was calculated using the energy balance between the macro scale measured experimentally and the local scale calculated numerically using a hierarchical multiscale constitutive damage to fracture law. A multi-scale image-based FEM model reconstructed from μCT imaging of the tissue and confocal microscopy at the cell scale. The model was subjected to experimental boundary conditions. The tissue mechanical properties are determined by correlating grey levels to nano-indentation measurements while confocal immuno-fluorescent microscopy measured the released chemicals by the cells under mechanical loading. The bone-on-chip mechanically behaved as fresh human bone. The cells reorganized in vitro as they would in vivo at the different stages of differentiation. The bone-on-chip produced after 109 days an ECM of which the strength was nearly a quarter of native bone, contained type I collagen at 256 days and was mineralized at 39 days. The cytoplasmic calcium concentration variations seemed to adapt to the expected in vivo mechanical load at the successive stages of cell differentiation. The systems were functional and allowed osteoconduction, osteoinduction and osteogenicity monitoring up to 567 days. Acknowledgements: With the support from NSF CMMI BMMB 1214816, the Farman Institute, the Fulbright Foundation. References: E. Budyn, M. Bensidhoum, S. Sanders, E. Schmidt, P. Tauc, E. Deprez, H. Petite, Bone-on-chip to study osteocyte mechanotransduction and ECM formation, European Cell and Materials, vol. 32, Suppl.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Computational Systems Mechanobiology for Dermal Wound Healing

Author(s): *Adrian Buganza Tepole, *Purdue University*.

Achieving perfect regeneration after injury has remained a challenge despite the growing understanding of the wound healing mechanisms and accumulation of experimental data on the matter. The fundamental gap arises from an overall result that cannot be inferred simply by adding up the parts. Rather, wound healing involves a well-coordinated interplay among different cell types, cell signaling networks and mechanical feedback loops evolving in space and time. Here we present a computational framework to study healing dynamics using continuum mechanics and computational systems biology. At the tissue scale we solve for tissue displacements that satisfy linear momentum balance, and cells and chemical concentrations which obey mass balance laws. At the cell scale we consider differential equations for growth and remodeling. The numerical implementation of our framework is done with in-house finite element code. In this work we consider two-dimensional geometries. The cell density field combines the effect of both fibroblasts and myofibroblasts. The chemical field lumps the action of inflammatory cytokines such as TGF-beta. The microstructure is defined by variables for permanent contraction, collagen mass fraction, and collagen alignment. Fibroblasts migrate following Keller-Segel chemotaxis and proliferate following logistic growth and upregulation with Michaelis-Menten kinetics due to the inflammatory signal [1,2]. Collagen production by fibroblasts is dependent on TGF-beta. We include an active stress to model how myofibroblasts exert traction on the tissue, driving wound contraction [3]. We model a square domain of 100x100mm, and create circular wounds of 20mm in diameter at the center. The wound is defined by lack of collagen and fibroblasts, and the initial condition for the wound domain is a spike in TGF-beta. The active stress driving wound contraction depends on the myofibroblast density, collagen content, and the chemical signal. Thus, and in agreement with recent experiments [3], the wound contracts primarily in a ring in the periphery of the disrupted tissue as the cells migrate in and the chemokines diffuse out of the wound domain. In conclusion, this model describes coupled chemo-bio-mechanical systems which allows investigation of the dynamics of wound healing based on mechanistic considerations. Further work is needed for calibration against experimental data and extension to more cell types and more sophisticated regulatory networks. [1] Buganza Tepole A. Comput Method Appl Mech Eng. 2017; 314(1):46-70. [2] Ronen M et al. Proc Natl Acad Sci U S A. 2002;99(16):10555-60 [3] Schmidt BA, Horsley V. Development. 2013;140(7):1517-27

14th U.S. National Congress on Computational Mechanics
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Title: Multiple Program Multiple Data FSI Coupling of Structural Dynamics (Sierra/SD) and UNDEX (NEMO)

Author(s): *Gregory Bunting, Scott Miller, *Sandia National Laboratories*; Jonathan Stergiou, *NSWC Carderock Division*.

Sierra/SD is a production structural dynamics code developed and maintained at Sandia National Laboratories. NEMO is a production underwater explosion (UNDEX) simulation code developed and maintained at NSWC Carderock Division. A fluid structure interaction (FSI) algorithm was implemented to facilitate coupling communication between the codes. The algorithm is based upon communication flags which permit each code to request certain actions, e.g., time step advancement, information passing, or output generation, from the other. Communication is done in an all-to-all pattern via MPI in a multiple program, multiple data (MPMD) model. Results presented include a 465-processor coupled analysis run of a large U.S. Navy surface ship with over 3 million structural elements and nodes and 25 million fluid elements. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL850000.

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Title: Short Fiber Reinforced Thermoplastic Composite Modelling Using Full Field Computing, Application to Glass Fiber Reinforced PEEK

Author(s): *Boris Burgarella, Aurelien Maurel-Pantel, Noel Lahellec, Hervé Moulinec, Frédéric Lebon, *LMA (France)*; Jean-Luc Bouvard, Noelle Billion, *Cemef (France)*.

May it be for ecologic or economic matters, structure mass reduction has grown to be one of the important factors in their conceptions. Integrating composite materials in the design process seems to be a good way to reduce weight. On the one hand, long fiber composites are known for their good mechanical characteristics but one of their drawbacks is the process complexity in large scale production (in the automotive industry for example). Short fiber thermoplastics composites on the other hand can appear as an interesting alternative since they are a good compromise between simple process and good mechanical properties (they are processed with a classical thermoplastic injection method). With the growing usage of these materials, comes a necessity of being able to understand and predict their behavior. Therefore, this study focuses on the visco-elastic modeling of short fiber thermoplastics composites (PEEK matrix – Glass fiber reinforcement) under small strain. To achieve this, a full field homogenization method based on the resolution of equations in Fourier space (FFT – Fast Fourier Transforms) has been used [1]. This method is a direct concurrent to the usual finite elements method, but it present the advantage of having the microstructure defined on a regular grid, and having shorter calculation times. The matrix is modeled by a generalized Maxwell model[2]. Following Micro-CT observations in the sample materials given by Solvay the material is supposed transverse isotropic. Finally, the glass fiber behavior is defined as elastic. With the FFT method, Representative Volume Elements (RVE) were loaded with sinusoidal strains in a DMA-like (Dynamic Mechanical Analysis) virtual experiment thus allowing the reconstitution of the master curve in each direction. These results were then used to identify a macroscopic transverse isotropic behavior model. Then, different types of micro-structures were computed, varying the fiber volume ratio, orientation distribution, and length distribution. The results of these computations were used to build a meta-model predicting the composite behavior for every microstructure in the boundaries defined by the experimental data-set. [1] Moulinec, H and Suquet, P. (1998). A numerical method for computing the overall response of nonlinear composites with complex microstructure. Computer methods in applied mechanics and engineering 157, 69-94 [2] Michel, J.C. et al. (1999). Effective properties of composite materials with periodic microstructure: a computational approach. Computer methods in applied mechanics and engineering 172, 109-143

14th U.S. National Congress on Computational Mechanics
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Title: Determination of Explosive Yields Using Nonlinear Bayesian Regression

Author(s): *John Burkhardt, *US Naval Academy*.

Explosive yields are often estimated by comparing fireball radius-time data to simplified, one parameter, hydrodynamic shock models. Experimentation has shown that these models accurately describe fireball evolution and provide reasonable yield and uncertainty estimates. These calculations, however, require the specification of an empirical constant that is, admittedly, poorly defined, as well as several theoretical parameters based on an overly simplistic model of the phenomenon. One of these theoretical parameters, related to the scaling of time, has been shown to be inaccurate through more sophisticated modeling and analysis. Consequently, the fidelity of the yield estimates and the validity of their uncertainty can be called into question. As an alternative to this commonly performed one parameter fit, this work accomplishes yield estimates by fitting the radius-time data to the full, underlying six parameter hydrodynamic model, leaving the commonly assumed parameters and their uncertainties as unknowns to be determined. The fit is accomplished using a nonlinear Bayesian regression analysis. A description of the parameter's probabilistic structure is generated using a Markov Chain Monte Carlo simulation of the model's posterior distribution using a traditional Metropolis-Hastings algorithm. Model sensitivity to start parameters, model convergence and posterior predictive checking are performed to confirm the robustness of the fit. Comparison with the typically assumed parameters and previously estimated explosive yields show reasonable agreement, however, significant differences exist. Most notable is an improved match between the Bayesian estimate of the time scaling parameter and its more sophisticated theoretical prediction.

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Title: Topology Optimization of Origami Structures with Multi-Stability

Author(s): *Philip Buskohl, *Air Force Research Laboratory*.

Origami structures are 2D to 3D mappings that can be designed to confer novel mechanical attributes, including auxetic behavior, tunable stiffness and mechanical instabilities that arise from geometric nonlinearity. Such properties are desirable for a variety of applications, including deployable shelters, robotic actuation and energy absorbing packaging, and highlight the adaptation and multifunctional qualities of an origami approach. Mechanical instabilities in origami structures are of particular interest as these bifurcations can often occur quickly, creating a dynamic response of the structure that can be leveraged for switch or sensor applications. However, the discovery of origami structures with mechanical instabilities is challenging given the complex geometric nonlinearities and the large design space to investigate. To address this challenge, we have developed a topology optimization framework for discovering origami fold patterns that realize stable and metastable positions. A nonlinear implementation of the truss element model, with additional stiffnesses associated with folding, is utilized to accurately handle the geometric nonlinearities from large folding. The multi-objective performance-function targets both the desired stable positions and nonlinear loading profiles of specific vertices in the origami structure. Building on the previous work of single vertex multi-stability analysis, e.g. “waterbomb” origami pattern, we expand the solution set of multistable mechanisms to include multiple vertices, nonhomogenous stiffness distributions and a broader set of reference configurations. Collectively, these results enable an initial classification of geometry-induced mechanical instabilities and highlight future opportunities for improvement of the optimization technique.

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Title: The Material Point Method in Offshore Geotechnical Engineering

Author(s): *Markus Bürg, Andriy Andreykiv, Liang Jin Lim, *Plaxis bv*.

We present a newly developed material point method (MPM) that uses second-order finite element shape functions. The method employs a fully implicit Newmark time discretisation scheme for solving time-dependent problems. The use of second-order finite element shape functions improves the accuracy of the numerical solution and reduces the oscillation of stresses being caused by material points crossing cell interfaces. To reduce stress oscillations even further, we employ a Dual Domain Material Point (DDMP) [1] Method formulation that has been incorporated into our implicit second-order formulation. To make the DDMP formulation being applicable on all common shapes of elements, e.g., quadrilaterals, hexahedra, triangles, and tetrahedra, a new, more general formula for the coupling of a shape function's original gradient with a smooth gradient has been derived. To reduce the computational cost of MPM, we have developed a natural coupling between MPM and FEM such that only regions, where large deformations are expected, have to be discretised by MPM. In regions with only moderate deformations, a standard finite element discretisation is being used. This approach improves the performance of the material point method significantly. In addition to this natural FEM-MPM coupling, we also have developed an augmented Lagrangian level-set contact formulation that allows for frictional contact between a penetrating structure - being discretised by FEM - and the soil which is being discretised by MPM. We apply our implementation to realistic applications in offshore geotechnical engineering and presented some typical offshore engineering processes, such as underwater slope collapses, anchor installation and extraction, and monopile installation. [1] D.Z. Zhang, X. Ma, P.T. Giguere: Material point method enhanced by modified gradient of shape function, J. Comput. Phys., Vol. 230, pp. 6379-6398, 2011

14th U.S. National Congress on Computational Mechanics
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Title: A Splitting Algorithm for the Numerical Simulation of Sediment Transport in Free Surface Flows

Author(s): *Alexandre Caboussat, *Geneva School of Business Administration, University of Applied Sciences Western Switzerland, Geneva, Switzerland*.

Sediment transport is becoming a crucial question in hydraulic and environmental engineering. In addition to sharp interfaces. between immiscible phases such as water and air, the modeling of sediments introduces an additional miscible phase in the liquid with diffuse interfaces. Challenges range from the physical modeling of the poly-dispersed sediments, the design of appropriate numerical methods for the coupled model, to the large-scale three-dimensional simulation of reservoirs and lakes. We present a numerical model for the simulation of 3D poly-dispersed sediments transported in a water flow involving free surfaces between the liquid and the ambient air. The physical model is based on a mixture model for multiphase flows. The Navier-Stokes equations for incompressible non-Newtonian flow are coupled with the advection and vertical deposition of the particles' concentration, and a Eulerian approach for the tracking of the free surfaces. The numerical algorithm relies on an operator-splitting method that decouples diffusion, advection and sedimentation processes. A well-chosen mix of finite elements, finite volumes and characteristics methods are dedicated to each sub-step of the time evolution algorithm. A volume-of-fluid approach to track the free surfaces between water and air. A two-grid discretization allows to treat the diffusion phenomenon on an unstructured finite element mesh, and the advection and vertical sedimentation phenomena on a Cartesian grid. This computational, multi-grid, framework has been extensively validated in the literature without considering sediments. The new contribution of the introduction of sediments lies in the accurate modeling of a mix of miscible and immiscible phases, with both sharp interfaces and diffuse interface regions to track and compute. The numerical model is validated through numerical experiments. A comparison with experimental results in various situations for mono-disperse and poly-disperse sediments, and the calibration of deposition fluxes, are performed. Large-scale simulations in real-life topographies for dam retention lakes show the robustness and the industrial potential of the approach. This is joint work with M. Picasso, A. Mrad (EPFL, Switzerland), S. Boyaval (Université Paris-Est, France), and A. Masserey, G. Steiner (Ycoor Systems SA, Switzerland).

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Title: Three-Dimensional Elastic Modulus Reconstruction Based on Magnetic Resonance Imaging

Author(s): *Luyao Cai, *Purdue University*; Claus b.w. Pedersen, *Dassault Systèmes Deutschland GmbH*; Corey p. Neu, *University of Colorado Boulder; Purdue University*.

Based on the displacements data measured by the dualMRI technique (displacements under applied loading by Magnetic Resonance Imaging), we reconstructed both two dimensional and three dimensional distribution of stiffness for internal tissue structure nondestructively. In the experiments, a bi-layer agarose gel was used to represent the complex gradient architecture of articular cartilage. Usually the traditional magnetic resonance elastography (MRE) is not able to assess cartilage stiffness due to the dissipation of high frequency shear waves in the human body, which is required to measure properties in thin and stiff cartilage. However, with the dualMRI technique, we are able to directly measure cartilage deformation under physiological cyclic loading. After the displacement data was collected, the spatial distribution of the elastic parameter was determined using topology optimization, which is a widely used non parametric optimization method for stiff, durable and light-weight structures design. Instead of maximizing the structure stiffness, as is used in traditional applications, here we applied topology optimization to determine the stiffness distribution by minimizing the absolute difference between experimental measured displacements and the finite element model. This process was accomplished using finite element method software Abaqus and optimization software Tosca (Dassault Systèmes). It was observed that the stiffness configurations both in 2D and 3D were restored. Since measurements and modeling can be done in three dimensions, no plane stress or plane strain assumption was required. It provided a nondestructive tool to measure the stiffness distribution of articular cartilage, and could help to reveal the pathogenesis or monitoring the healing process of osteoarthritis, in which the stiffness of articular cartilage decreases.

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Title: Nonlinear Dynamic Analysis of Space Tethered Solar Power Station

Author(s): Xuefu Li, *DalianUniversity of Technology*; *Zhiqin Cai, Jinying Wu, *Dalian University of Technology*.

The nonlinear dynamics of the space tethered solar power station is presented. Dynamical formulations are developed for the solar power station system which consist of two main parts: the bus system and the solar power panel. The orbital motions of the system, the rotation of the solar power panel, the deployment/retrieval of tethers and the vibration of tethers are taken into account. The dynamics behavior of the tethered space solar power station is researched by numerical simulation. Without any disturbance, the on-orbit movement of tethered space solar power station is simulated, then the stability analysis is carried out with different kinds of disturbances. Influences of initial attitude errors of the solar power panel, tether's longitudinal and transverse vibrations on the bus system and the solar power panel are analyzed. The numerical results demonstrate that some disturbances have significant impact on the system.

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Title: Profiling AMR/C Computations in MontBlanc Exascale Prototype

Author(s): *Fabio Canesin, *Schlumberger*; Jose Camata, Alvaro Coutinho, *COPPE/UFRJ*.

With the ever increasing requirements of modeling complexity and high-fidelity results, High-Performance Computing (HPC) is expected to continue to expand its role in computational mechanics. Several system architectures are currently being proposed in the quest for the Exascale level of performance with increased power efficiency. This paper presents a performance profiling of an adaptive mesh refinement and coarsening finite element solver on the Mont-Blanc project prototype. Built on leveraging current state-of-the-art scientific libraries libMesh and PETSc, the solver evaluate the performance behavior of established software on a new HPC architecture making use of the ARMv8 system on a chip (SoC) processors. The transient solution of the incompressible Navier-Stokes equations are used as benchmark and scalability of the solver is evaluated on a test system built with the 48-core ThunderX SoC. The same profiling is performed on the Lobo Carneiro system built with a conventional HPC architecture based on Xeon processors and InfiniBand interconnect. Comparative performance characteristics of the Mont Blanc relative to Lobo Carneiro are drawn.

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Title: A Posteriori Error Estimation and Adaptivity for the Virtual Element Method

Author(s): *Andrea Cangiani, Oliver J. Sutton, *University of Leicester (UK)*; Emmanuil H. Georgoulis, *University of Leicester (UK) & NTUA (Greece)*; Tristan Pryer, *University of Reading (UK)*.

We present a posteriori error analyses for the Virtual Element Method [1,2] applied to elliptic [3] and parabolic (in preparation) problems. The resulting error estimators are of residual-type and apply on very general polygonal/polyhedral meshes. The estimators are fully computable as they rely only on quantities available from the Virtual Element solution, namely its degrees of freedom and element-wise polynomial projection. The error estimators are used to drive adaptive mesh refinement in a number of test problems, including reaction-diffusion systems relevant to cyclic competition models from mathematical biology. Mesh adaptation is particularly simple to implement since elements with consecutive co-planar edges/faces are allowed and, therefore, locally adapted meshes do not require any local mesh post-processing. Furthermore, the extreme generality of the meshes allowed opens the way to endless possibilities on how one may refine and coarsen. The design of adaptive algorithms able to exploit such flexibility is, however, a non-trivial task and something that we just started to explore. [1] L. Beirao da Veiga, F. Brezzi, A. Cangiani, G. Manzini, D.L. Marini and A. Russo. Basic principles of Virtual Element Methods. M3AS, Vol. 23(1), 199–214, 2013. [2] A. Cangiani, G. Manzini, and O. Sutton. Conforming and Nonconforming Virtual Element Methods for Elliptic Problems. IMAJNA online, 2016. [3] A. Cangiani, E. H. Georgoulis, T. Pryer, and O. Sutton. A Posteriori Error Estimates for the Virtual Element Method. Submitted for publication.

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Title: High-Order Mesh Generation and Flow Simulation about Complex Geometries

Author(s): *Chris Cantwell, Mike Turner, Joaquim Peiro, Spencer Sherwin, *Imperial College London*; David Moxey, *Exeter University*; Ayad Kassim, *Hwelett Packard Enterprise*.

We will describe our latest efforts in simulating complex flows about realistic geometries using high-order unstructured spectral/hp elements. We will discuss the developments in mesh generation [1] and flow solution [2] that have led us to successfully simulate flows about geometries as complex the Elemental RP1 track car. We believe this is the first high-order flow simulation for an automotive whole car geometry, and certainly one of the most complex geometries that has ever been attempted by this method. The computational domain is discretized into approximately 2.5 million cells (tetrahedra and prisms), of spectral methods with 5th order polynomials, approximately one billion degrees of freedom, required to represent the flow features to the desired accuracy. The flow Reynolds's number is 50,000 and the boundary layer is captured using a layer of prisms close to the surface to the car. [1] C. D. Cantwell, et al., "Nektar++: an open-source spectral/hp element framework," Computer physics communications, 192 (2015) 205–219. [2] M. Turner, J. Peiro, D. Moxeya, A variational framework for high-order mesh generation, Procedia Engineering 163 (2016) 340–352

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Title: An Embedded Robin Boundary Method for Incompressible Fluid-Structure Interaction Problems with Large Deformation

Author(s): *Shunxiang Cao, Kevin Wang, *Virginia Tech*; Alex Main, *Duke University*.

Partitioned procedures are widely used in the solution of fluid-structure interaction (FSI) problems, primarily because they facilitate the use of advanced numerical algorithms and computational codes developed specifically for each sub-system. However, numerical instability is a key issue, especially when the fluid is incompressible. In this paper, we present a numerically stable partitioned procedure featuring a parameter-free Robin-Neumann interface condition and an embedded boundary method. First introduced in [Badia, Nobile and Vergara, J. Comput. Phys. 227, 2008], the one-parameter Robin-Neumann interface condition has been shown to significantly mitigate the numerical added-mass effect when the model parameter introduced to the Robin interface condition is carefully selected. In this work, we apply this approach to an embedded boundary method for FSI problems with complex geometry, large structural deformation, and/or topological change (e.g., fracture). Specifically, we first establish a two-dimensional FSI model for which the analytical solution can be derived in closed-form formulation. Using this model, we analyze the effect of the aforementioned model parameter to numerical stability and accuracy, and derive its optimal value. Next, we present the numerical algorithms to enforce the Robin-Neumann interface condition for general incompressible FSI problems, in the context of embedded boundary method. In particular, this new computational framework is equipped with a fluid solver based on hybrid approximate projection method in which operator splitting of Robin interface condition is used to construct appropriate boundary conditions for advection-diffusion step and projection step. To enforce boundary conditions at embedded interface for each step, a Ghost-cell method and Shortley–Weller embedded finite-difference method are used. The model parameter in the Robin boundary condition will be determined locally based on evaluating the simplified FSI model mentioned above. The salient features of the proposed numerical method will be assessed using the widely-used Turek-Hron benchmark problem and several model problems in the context of bio-inspired aerial and aquatic propulsion.

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Title: Developing SPH Based Modeling of Volcanic Plumes Using Modified SPH Schemes

Author(s): *Zhixuan Cao, *University at Buffalo*; Abani Patra, *University at Buffalo, SUNY*.

VATDs (Volcanic ash transport and dispersion models) used for critical volcanic ash forecasts usually take outputs of eruption plume models as source terms. The accuracy of source terms is crucial for forecasts from such VATDs. All existing 3D (three dimensional) plume models described in the literature use mesh based methods. SPH (Smoothed particle hydrodynamics), as a mesh free method has several advantages over mesh based methods in modeling of multiphase free boundary flow. As an initial effort on exploiting 5 the feasibility and advantages of SPH in volcano plume modeling we adopt a relatively simpler model, a 3D dusty-gas dynamic model, targeted at capturing the salient features of volcano plume. In this model, erupted material is assumed to be well mixed and represented by one phase while air is another phase. We also assume immediate dynamic and thermal dynamic equilibrium between air and erupted material and that the effect of wind is not significant. Several newly developed techniques in SPH are adopted and extended to address numerical challenges in simulating multiphase compressible turbulent flow with classical SPH method. The SPH "turbulence model is adopted to capture mixing at unresolved scales. Heat exchange due to turbulence is then calculated with Reynolds analogy. Corrected formalism of SPH is used to handle tensile instability and deficiency of particle distribution near the boundaries. We also propose feasible ways to impose velocity inlet and pressure outlet boundary conditions, both of which are scarce in traditional implementations of SPH. The core solver of our model is parallelized with MPI (message passing interface) obtaining good weak scalability and strong scalability. The model is first verified by comparing velocity and concentration distribution along axis and cross section with experimental results of JPUE (jet or plume which is ejected from a nozzle into a uniform environment). The top height of Pinatubo eruption (15 June 1991) simulated by our model is consistent with both observation and existing 3D plume models. Profiles of several integrated variables are compared with these by existing 3D plume models and further verifies the correctness of our model. Analysis on the plume evolution process illustrated that this model is able to reproduce the basic physics of plume development. The comparison also implies that turbulence model plays a significant role in 3D volcano plume modeling. We also experiment with Godunov SPH schemes to better capture plume-atmosphere interfaces.

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Title: Structure-Preserving Model Reduction for Finite-Volume Discretizations of Conservation Laws

Author(s): *Kevin Carlberg, Youngsoo Choi, *Sandia National Laboratories*; Syuzanna Sargsyan, *University of Washington*.

Finite-volume discretizations are commonly used for numerically solving systems governed by conservation laws, especially those appearing in compressible fluid dynamics. Such techniques numerically enforce conservation laws over cells by discretizing the integral form of the conservation laws. However, such models can become very large-scale for when high fidelity (i.e., high spatial resolution) is required, leading to simula- tion times that can exceed weeks on a supercomputer. As a result, these high-fidelity models are not practical for many-query and real-time scenarios such as model predictive control and uncertainty quantification. Reduced-order models (ROMs) have been developed to mitigate this burden. However, most techniques in the literature have focused on generating ROMs for finite-element discretizations of conservation laws (e.g., Refs. [2,3]). While some techniques like the Gauss–Newton with approximated tensors (GNAT) method [1] have been successfully applied to finite-volume models, these techniques do not guarantee that conservation laws are enforced over any subset of the computational domain. As a result, instability and inaccurate responses are common; even responses with low errors generally yield spurious generation or dissipation of quantities that should be conserved. To address this, we propose a nonlinear model-reduction technique that explicitly enforces conservation laws over subdomains of the problem. This guarantees that, even when the dimensionality of the model is greatly reduced, the most important structure intrinsic to the finite-volume model—the conservation laws—are enforced over subdomains. We refer to the method as the GNAT-finite volume (GNAT-FV) technique, as it amounts to equipping the nonlinear least-squares GNAT formulation with equality constraints associated with conservation laws over subdomains. Furthermore, we equip both the objective function and constraints with hyper-reduction via gappy POD; this ensures computational efficiency in the presence of nonlinearities. Numerical results highlight the improvement in long-time behavior of GNAT-FV over existing ROMs (i.e., Galerkin, least-squares Petrov–Galerkin, and GNAT) when applied to finite-volume models. References: [1] K. Carlberg, C. Farhat, J. Cortial, and D. Amsallem. The GNAT method for nonlinear model reduction: effective implementation and application to computational fluid dynamics and turbulent flows. Journal of Computational Physics, 242:623–647, 2013. [2] G. Rozza. Reduced basis methods for Stokes equations in domains with non-affine parameter depen- dence. Computing and Visualization in Science, 12(1):23–35, 2009. [3] K. Veroy and A. T. Patera. Certified real-time solution of the parametrized steady incompressible Navier-Stokes equations: Rigorous reduced-basis a posteriori error bounds. International Journal for Numerical Methods in Fluids, 47(8):773–788, 2005.

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Title: Topology-Optimized Design of Architected Materials with Multiple Materials

Author(s): *Josephine Carstensen, James Guest, *Johns Hopkins University*.

Recent advances in manufacturing technologies, including additive manufacturing, has made it possible to realize increasingly complex architected materials. This has created demand for new design methods, drawing attention to computational design tools such as topology optimization. Topology optimization of material has previously been used with a single solid material to obtain designs with a range of improved performance properties, including mechanical, thermal and fluidic properties such as maximized bulk-, Young's- and shear modulus, design of negative Poisson's ratio materials, and maximized thermal conductivity and fluid permeability. For materials design problems an upscaling law is required to relate the unit cell behavior to the effective material properties. Numerical homogenization is typically used for elastic design. The topology optimization formulation presented herein uses an existing SIMP based multi-material design and sensitivity scheme [1] as the back-bone of the algorithm. When optimizing for nonlinear objectives to include material plasticity and geometric nonlinearities, we use the existing sensitivity formulations [2,3] and use finite periodicity due to the lack of a recognized homogenization technique. The optimization is performed using MMA as the gradient based optimizer and the manufacturability of the design is improved by ensuring minimum length scale control through the Heaviside Projection Method. Several topologies will be shown including designs for multi-objectives in mechanical and thermal properties. In this context, architected materials refer to periodic materials with a representative unit cell that is repeated throughout. References: [1] Gaynor et al., Journal of Manufacturing Science and Engineering, (2014). [2] Maute et al., Structural Optimization, (1998). [3] Buhl et al., Structural and Multidisciplinary Optimization, (2000).

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Title: Divergence-Conforming and Fully-Implicit Simulation of Cell-Scale Blood Flow

Author(s): *Hugo Casquero, Yongjie Zhang, *Carnegie Mellon University*; Carles Bona-Casas, *Universitat de les Illes Balears*; Hector Gomez, *Purdue University*.

The mechanical behavior of blood depends on the scale under study. In large vessels with a diameter greater than 500 μm, treating blood as a Newtonian fluid with constant viscosity is accurate enough for most applications. Nevertheless, in vessels with smaller diameters, blood behaves clearly as a non-Newtonian fluid. An appealing option to simulate microscale blood flow is to at least consider explicitly blood plasma and red blood cells (RBCs), which leads to a fluid-structure interaction (FSI) problem in which both RBCs and blood plasma are incompressible. After successive enhancements of our immersed method for FSI [1-3], we have come up with a method that is inf-sup stable, pointwise divergence-free, and fully-implicit in time. We have also developed a scalable implementation of our method which is mandatory in order to tackle the challenging application of cell-scale blood flow. We will study the flow patterns and rheology of blood in normal and stenosed arterioles. The stenosis of arterioles can lead to important diseases as coronary microvascular disease and lacunar infarct. The flow characteristics of stenosed arterioles are quite different from those of macrovascular stenosis due to the fact that blood behaves as a Newtonian fluid in large arteries, but as a non-Newtonian fluid in arterioles. Finally, we will show the effects of size, deformability, and density when it comes to islolate nucleated cells from blood samples using mechanical means. REFERENCES [1] H. Casquero, C. Bona-Casas, H. Gomez, A NURBS-based immersed methodology for fluid-structure interaction. Computer Methods in Applied Mechanics and Engineering, 284, 943-970, 2015. [2] H. Casquero, L. Liu, C. Bona-Casas, Y. Zhang, H. Gomez, A hybrid variational-collocation immersed method for fluid-structure interaction using unstructured T-splines. International Journal for Numerical Methods and Engineering, 105, 855-888, 2016. [3] H. Casquero, C. Bona-Casas, H. Gomez, NURBS-based numerical proxies for red blood cells and circulating tumor cells in microscale blood flow. Computer Methods in Applied Mechanics and Engineering, 316, 646-667, 2017.

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Title: Mimetic Discretization Methods for Solving Electrical Conduction Problems in Laminated Composites with Cracks

Author(s): Luis waldo Escalona galvis, *Computational Science Research*; Johnny Corbino, Satchi Venkataraman, *Jose Castillo, *Computational Science Research Center, San Diego State University*.

Carbon fiber reinforced polymer (CFRP) composites are preferred materials in the aerospace industry due to their outstanding mechanical stiffness and strength properties. Intralaminar matrix cracking and interlaminar delamination failure are common damage modes present in CFRP composites. Internal damage interrupts inner electrical paths that create changes in resistance measurability using Electrical Resistance Tomography (ERT). ERT reconstructs the internal electric behavior of the material by measuring electric potentials on the boundaries when electric current is injected. Damage identification uses inverse identification algorithms that minimize the difference between the measured change in electrical properties at surface electrodes and the model predicted values for the same. The model is the forward solution to the electrical conduction problem governed by Laplace's equation of the electric potential, for specified electrical conductivity distribution in the domain and boundary conditions. Mimetic discretization methods [1] have been used for the solution of the diffusion equation [2] and its convergence has been proved on rough logically-rectangular grids with convex cells [3]. Nonetheless, the numerical solution of the forward problem for a composite in the presence of discontinuities due to cracks represents a challenge. The present work explores the use of mimetic discretization methods for the electrical conduction problem in thin layered materials with orthotropic properties and embedded cracks. We solve a diffusion equation for a 3D model of a thin laminate with applied electric current. In the model we apply Dirichlet and Neumann boundary conditions on the electric potential and the electric current respectively. We use second order accurate discrete gradient and divergence operators. Material orthotropy is accounted for by changing the conductivity tensor properties at each ply. Delamination cracks are modeled by locally changing electric conductivity in the across-the-thickness direction where the affected interlamina is located. Different crack locations and sizes are considered. Damage cases show the highest sensitivity as it is expected in ERT applications. The results show the effectiveness of using mimetic methods in modeling composite laminates for damage detection using Electrical Resistance Tomography. References: [1] Castillo, J. and Miranda G. (2013). Mimetic Discretization Methods. United States: CRC Press. 230p. [2] J. Hyman, J. Morel, M. Shashkov, and S. Steinberg. Mimetic finite difference methods for diffusion equations. Technical Report LA-UR-01-2434, Los Alamos National Laboratory, Los Alamos, New Mexico, 2001. [3] Hyman J. and Steinberg S. (2004). The Convergence of Mimetic Discretization for Rough Grids. Computer and Mathematics with Applications, 47, pp. 1565-1610.

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Title: Characterization of Self-Coalescence in Microfluidic Capillary Flow via Finite Element Method

Author(s): *Samuel Castonguay, Thomas Gervais, *Polytechnique Montréal, CANADA*; Onur Gökçe, Yuksel Temiz, Emmanuel Delamarche, *IBM Research – Zurich, SWITZERLAND*.

Reagents delivery and flow control in microfluidic modules is ubiquitous in BioMEMS applications [1]. Although the dynamic of dispersion in microchannels is well established, generating custom patterns with specific concentrations of wetted reagents still proves to be difficult and often implies complex two-phase or surface driven flows, which are difficult to model numerically. Recently, Gökçe et al [2] have proposed a general method to increase control over reagent resuspension by geometrically confining a water droplet in a capillary microstructure and forcing it to "fold" onto itself in a process called "self-coalescence" (SC). Understanding reagent transport in SC requires solving the Navier-Stokes equation in two-phase flow with moving interfaces, a well-known, challenging problem in computational fluid dynamics (CFD). One could use tracking methods [3], by which the mesh moves to track the interface or a flow-interface system is solved on a static mesh. However they prove to be computationally intensive and tedious to implement. Instead, in the case of self-coalescing flows we provide a simple approach to characterize these types of flow in elongated structures such as microfluidic channels. To simplify the problem, we first numerically validate that capillary flows inside a shallow microfluidic channel can be approximated as a flow in a Hele-Shaw cell. Then, we show that the system can be numerically modeled in the reference frame of the moving air/water interface to regularize boundary conditions. Finally, we compared solutions obtained via Finite Element Modeling (FEM) with experimental results of self-coalescing flows as well as with asymptotic analytical models obtained via conformal mapping. Simulations show great correlation with experimental microPIV data and asymptotic analytical models. Furthermore, our numerical results indicate that self-coalescence flows can withstand large variations of contact angles and depend only slightly on the type of wetting barriers used. It is thus a very useful tool to optimize device design and operation. The suggested method is not computationally demanding and could be used to study a variety of two-phase flows involving moving boundaries in elongated, shallow flow cells containing obstacles. REFERENCES: 1. Hitzbleck, M. & Delamarche, E. Reagents in microfluidics: an 'in' and 'out' challenge. Chem Soc Rev 42, 8494–516 (2013). 2. Gökçe, O. et al. Passive "orthogonal flow mixers" for homogeneous dissolution of reagents in microfluidics. MicroTAS (2016). 3. Tezduyar, T. E. Finite element methods for flow problems with moving boundaries and interfaces. Arch Computat Methods Eng 8, 83–130 (2001).

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Title: Development of a Fracture Tip Plastic Zone in Semi-Consolidated Sedimentary Rock Georeservoirs During Hydraulic Fracture Propagation

Author(s): *Robert Caulk, Ingrid Tomac, *Univ. Calif., San Diego*.

Hydraulic fracture propagation within semi-consolidated sandstone rock is modeled using the Discrete Element Method (DEM) implemented within YADE open source code. The DEM model implements a modified Mohr-Coulomb criterion for particle bond breakage combined with a compressible Pore-scale Finite Volume scheme and permeability step function to approximate the behavior of semi-consolidated sandstone during hydraulic fracture propagation. Specifically, the hydro-mechanical coupling enables the micromechanical investigation of the dynamic plastic zone ahead of the fracture tip. Results show that the development of this plastic zone reflects the porous and compliant structure of the rock matrix. Just beyond the fracture tip, high rock permeability enables fluid invasion and increased pore pressures, which lead to reduced effective stresses where stresses are already concentrated. This paper investigates effects of stresses and the semi-consolidated nature of the rock on the shear failure and a collapse of the matrix. The high crustal pressures may lead to poroelastic behavior and plasticity of the fluid-rock structure.

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Title: Direct Energy Deposition Simulation Using Truchas

Author(s): Neil Carlson, *Ondrej Certik, *LANL*; Terry Haut, *LLNL*.

Metal casting and additive manufacturing processes are designed to yield material with desired characteristics (microstructure, porosity, defects, etc.), which determine its properties. Computational modeling is an important tool in understanding this process-to-structure link, and in guiding the design of these processes. We will describe direct energy deposition additive manufacturing process implementation using LANL's parallel casting code Truchas [1], which includes coupled models for free-surface incompressible fluid flow, heat transfer, and solidification. Using these modules Truchas is able to model the weld pool as well as the melting and solidification process as a coupled problem. In this talk we will describe the details of the computational model and validation with existing experimental data. [1] https://gitlab.com/truchas/truchas-release LA-UR-17-22147

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Title: Certified Computations with PGD Model Reduction in the MsFEM Framework

Author(s): *Ludovic Chamoin, *ENS Paris-Saclay*; Frédéric Legoll, *ENPC*.

The Multiscale Finite Element Method (MsFEM) is a powerful numerical method in the context of multiscale analysis. It uses basis functions which encode details of the fine scale description, and performs in a two-stage procedure: (i) offline stage in which basis functions are computed solving local fine scale problems; (ii) online stage in which a cheap Galerkin approximation problem is solved using a coarse mesh. In this framework, we recently proposed an a posteriori error estimate using the concept of Constitutive Relation Error (CRE) based on dual analysis. It enables to effectively assess the various error sources, and to drive a robust adaptive algorithm. In the present work, we wish to investigate the additional use of model reduction inside the MsFEM strategy in order to further decrease numerical costs. We particularly focus on the use of the Proper Generalized Decomposition (PGD) for the computation of multiscale basis functions. PGD is a suitable tool that enables to explicitly take into account variations in geometry, material coefficients, or boundary conditions. In many configurations, it can thus be efficiently employed to solve with low computing cost the various local fine-scale problems associated with the MsFEM approach and its verification a posteriori. We will show performances of the coupling between PGD and MsFEM on several applications in which the microstructure is parametrized. and we will define dedicated estimates to certify the quality of the overall MsFEM solution.

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Title: Strong C1 Coupling of Multi-Patch 3D PHT-Splines

Author(s): *Chiu Ling Chan, Cosmin Anitescu, Timon Rabczuk, *Bauhaus-Universität Weimar*.

A key feature of isogeometric analysis is that it integrates the modeling and analysis process by employing compatible spline function spaces (such as NURBS). The p-degree spline functions allow up to C^{p-1} continuity within each patch. However, when modeling complex shapes, it is necessary to couple multiple patches together. It is a challenging task to obtain global continuity beyond C^0 on the multi-patch geometries. Recently, a C^1-smooth coupling on planar bilinear multi-patch domains has been presented in [1]. It would be appealing to have a general framework for strong patch coupling in higher dimensions and for arbitrary domains. In this work, we present the coupling of multi-patch polynomial splines over hierarchical T-meshes (PHT-splines) [2] in 3D domains with C^1 continuity. The main idea is to impose C^1 continuity constrains to the graph surfaces of the isogeometric functions along the common interfaces. In addition to the benefit of local refinement inherent to hierarchical bases, we overcome C^1 locking by performing partial degree elevation on the elements along the patch interfaces. Thus, the computational cost is reduced significantly compared to elevating the degree of all basis functions. This method is tested for 3D shell objects, and the results obtained show the potential of the presented method for modeling and analysis of complex geometries. References [1] M. Kapl, F. Buchegger, B. Bercovier, B. Juttler, Isogeometric analysis with geometrically continuous functions on planar multi-patch geometries. Comput. Methods Appl. Mech. Engrg. 316 (2017) 209-234. [2] J. Deng, F. Chen, C. Hu, W. Tong, Z. Yang, Y. Feng, Polynomial splines over hierarchical T-meshes. Graphical Models. 70 (2008) 76-86.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Time-Domain Multi-Patch Discontinuous Galerkin Methods

Author(s): *Jesse Chan, *Rice University*; John Evans, *UC Boulder*.

We consider IGA methods within the context of explicit time-stepping schemes, which require the inversion of a mass matrix at each time step. Higher dimensional discretizations possess a tensor product construction over a given patch; however, while this structure can reduce costs for assembling or applying finite element matrices in higher dimensions, it does not carry over to the mass matrix inverse due to the presence of geometric weightings. This lack of a tensor product structure greatly increases the cost of explicit time-stepping. In this talk, we show how a "weight-adjusted" approximation to the inverse mass matrix recovers the tensor product structure on a single patch while retaining provable energy stability and high order accuracy. Geometric flexibility and computational efficiency are achieved by coupling patches together using a multi-patch discontinuous Galerkin discretization.

14th U.S. National Congress on Computational Mechanics
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Title: Mechanical Properties of Rhenium Disulfide and Rhenium Diselenide: A First-Principles Study

Author(s): *Pratyaksh Agrawal Chandra veer Singh, *University of Toronto*.

Transition metal dichalcogenides (TMDs) have recently attracted a large interest due to their unconventional and unique electronic and optical properties. Most of the TMDs have a graphene like hexagonal crystal structure that consists of metal atoms (M) layers sandwiched between chalcogen atoms (X) and have MX2 stoichiometry. Rhenium disulfide (ReS2) and diselenide (ReSe2) are a new member of 2D TMDs semiconductors, which have been successfully fabricated recently 1. Unlike hexagonal TMDs, ReX2 (X= S, Se) are direct band-gap semiconductors (1.5-1.6 ev) in the bulk and do not show any further transition when confined to monolayer form 1. ReX2 have unique electrical and optical properties like, in-plane anisotropy, quasi-direct band gap, small dipole moment and weak binding energy. Despite the significant progress in experimental and theoretical investigation of ReX2 , mechanical properties of these two materials have not been fully studied yet. In this work, we have performed extensive density functional theory calculations to evaluate the mechanical properties of ReX2 and compared them with graphene. Our simulation results showed that for ReX2, nonlinear relationship exists between stress and strain. Additionally, we noticed that strain softening takes place for lagrangian strains larger than 10%. It was found that in ReS2 Young's modulus, ultimate tensile strength (UTS) and strain corresponding to UTS during uniaxial tension in x direction are larger than that of ReSe2 . We have also determined a complete set of nonlinear anisotropic elastic constants up to the fifth order for ReX2 using the assumptions of continuum mechanics by fitting the stress-strain responses under uniaxial and biaxial tension until the point of fracture. Our calculations predicted that ReS2 has larger C11 than that of ReSe2 . This observation is in agreement with our previous result which revealed that ReS2 has larger young modulus and UTS than ReSe2 . Also, we have used charge density plots and virtual Scanning Tunneling Microscopy images to analyse the initiation of fracture under uniaxial and biaxial tensile loading in these two structures.

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Title: Limited-Memory Finite Element Simulation of Fused Deposition Modeling Process

Author(s): *Aaditya Chandrasekhar, Buzz Rankouhi, Krishnan Suresh, *UW, Madison*.

Fused deposition modeling (FDM) is one of the most widely adapted Additive Manufacturing (AM) processes, which involves layer-by-layer deposition of a thermoplastic polymer. The layer-manufacturing nature of this process along with intensive heat, and rapid cooling of the polymer can cause warpage, delamination of layers, and deviation from the original design geometry, resulting in low print reliability and repeatability. Shop floor experimentation can be expensive and time consuming. An accurate, fast and reliable simulation of the FDM process can help alleviate this issue. While there have been significant strides in understanding the underlying physics, there has been less notable progress in increasing the efficiency of the simulation. To effectively simulate the thermo-mechanical printing process, current strategies require a massive computation power, which makes it time and cost ineffective. In this study, we propose a novel limited-memory framework using assembly free finite element method to simulate the thermo-mechanical phenomena during FDM process, followed by physical testing. The proposed framework showed a significant speedup in the simulation without loss of accuracy. This framework can be easily adapted to other AM techniques that involve material deposition. Furthermore, in situ temperature measurements were carried out to verify the temperature gradient during the FDM process. Different prototypes were fabricated and distortions due to residual stresses were measured to be compared with simulation results.

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Title: The Thermal Transport in Branched Carbon Nanotube

Author(s): *I-ling Chang, Yu-wei Lo, *National Cheng Kung University*.

Thermal management is a key issue in a lot of electronic devices. Carbon nanotubes (CNTs) with branches were found to be a potential candidate to rectify thermal energy while retaining electric conductance. Here, thermal transport behavior of branched CNTs was investigated using non-equilibrium molecular dynamics (NEMD) simulation method. The atomic model of CNTs with T junction was first equilibrated at 300K using Nose-Hoover thermostat. The interaction between carbon atoms were described using REBO potential and the simulations were performed using LAMMPS. Both symmetric and asymmetric temperature-controlled NEMD simulations were applied on the three branches of the CNT models to examine how the thermal energy transported. The effects of branch length and diameter were studied. Moreover, the thermal flux ratios between branches were calculated and compared with the theoretical prediction based on 1-D heat transfer assumption. It was clarified that ballistic and diffusive thermal transports play important roles in the energy transfer depending on the branch length. Besides, it was also concluded that the atomic defects, i.e., 7- or 8-membered rings, on the T junctions would impose anisotropic thermal conductance.

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Title: A Study on Dynamic Reduction Method for Acoustic Modal Analysis

Author(s): *Seongmin Chang, Kang-Heon Lee, Gyu Mahn Lee, Jong-Wook Kim, *Korea Atomic Energy Research Institute*.

Recently, the system-integrated reactor has been widely researched due to its natural advantages in structural integrity resulting from removing of pipelines between reactor pressure vessel and main components (e.g. reactor coolant pump, steam generator). This reactor design implies that the internal structures and main components should be located inside of pressure vessel resulting in complex arrangement and design. In the design of reactor pressure vessel, one of the main issues is performing the acoustic modal analysis to understand the dynamic characteristics of the structures which surrounded by reactor coolant. However, due to its complexity, considering not only the internal structures and main components but also the reactor coolant requires huge amounts of human and computational resources in time. In this research, the effective numerical method for acoustic modal analysis is proposed by adopting the dynamic reduction method which has been widely used for structural engineering. Future works on the acoustic harmonic analysis of internal structures will be briefly discussed.

14th U.S. National Congress on Computational Mechanics
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Title: The Structural Changes of Finger 3 in the Mutated Ankyrin Repeat Domain of the Human TRPV4 Channel Alter ATP Binding Ability

Author(s): Tsu-Hsin Kao, *Shu-Wei Chang, *National Taiwan University*.

Transient receptor potential channel subfamily V member 4 (TRPV4) is a calcium-permeable cation channel protein that plays a mechanosensory or osmosensory role in several musculoskeletal tissues. Recent studies have reported that TRPV4 is required for breast cancer cell invasion and transendothelial migration by reducing cell rigidity through controlling the cytoskeleton at the cell cortex. On the other hand, mutations in the TRPV4-ARD have been shown to cause many diseases. These findings suggest that TRPV4 plays an important role in human body and it is crucial to understand the fundamental mechanisms regulated by chemical ligands such as adenosine triphosphate (ATP) binding with the ankyrin repeat domain (ARD) of TRPV4. However, how these mutations at the molecular level result to the diseases is still unclear. The relationships between the regulatory interactions and the various kinds of diseases are also still not well understood. In this study, we investigate the molecular mechanisms of the ligand biding of the TRPV4-ARD by using molecular dynamics (MD) simulations. We construct the full atomistic models of the TRPV4-ARD with and without mutations to study the structural changes in normal and mutated TRPV4-ARD, especially in the Finger 3 of the TRVP4-ARD which is thought to be critical for the binding ability. The structural changes caused by the point mutations of the TRPV4-ARD at E183■K197 and L199 are analyzed. We find that the side chains of these amino acids fold into a particular way, determining the conformation of the protein. These conformational changes alter the flexibility of Finger 3 and the arrangements of aromatic residues in the Finger 2 and 3. Our results explain how these point mutations in the TRPV4-ARD could affect its binding ability with the ATP. This study provides fundamental insights into the mutation induced structural changes of the TRPV4-ARD and help to explain how the mutations alter the ATP-binding ability of TRPV4-ARD.

14th U.S. National Congress on Computational Mechanics
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Title: The Development of Numerical Method for Ship and Wave Interaction Analysis using NURBS

Author(s): *Keng-Wei Chang, Pai-Chen Guan, *National Taiwan Ocean Univ.*.

In general mesh-based analyzing processes, we always use CAD software, which construct geometry based on the B-spline function, to build geometrical model for engineering purposes. The geometrical model is later imported into the finite element method software, which will redundantly rebuild the model again with finite element mesh (discretization). This processes will make the error from approximation, and that some problem which sensitive to geometric (like the high order modal analysis) will lead to large error. The IGA directly uses B-spline as the shape function, so it can skip mesh generation. Because B-spline is a high order and high continuity function, it can build exact high order surface and analyze contact problems which need more differential time. We also build the analysis program according to the analysis procedure and do some test. We use a plate to calculate the natural frequency and compare with commercial software and exact solution and comfrime that IGA can converge quickly and has high accuracy in the high-order mode. Then, we do the dyanmic analysis and confirms that it can complie with the exact solution. After we complete the verification of the developed program with several benchmark problems, we apply this program to analyze the block structure and confirm that deformation behavior is reasonable. After sturacture analysis, we solve General Shallow Wave Equations with NURBS in order to efficiently simulate water flows on solid surfaces under shallow wave assumptions. Finall, We present a coupling method to model interactions between fluid and floating rigid objects.

14th U.S. National Congress on Computational Mechanics
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Title: Projection-Based Model Order Reduction for Nonlinear Contact Problems

Author(s): *Todd Chapman, Charbel Farhat, *Stanford University*.

Parametric studies of deformable structures through high fidelity simulations can be prohibitively computationally expensive. The expense is compounded when contact is modeled through non-penetration conditions. Furthering previous work on projection-based model order reduction with node-to-node contact [1], a complete workflow for constructing robust local Hyper Reduced-Order Models (HROMs) for comprehensive nonlinear contact problems is described in this presentation. The HROMs are based on the Energy Conserving Sampling and Weighting method [2] and must satisfy certain solvability conditions that will be discussed. The local Reduced-Order Basis (ROB) approach [3] is used to construct efficient ROBs for the primal and dual states, where the latter are used for non-penetration enforcement. Distinct physical regimes are identified through clustering and the dimensionality of the resulting local subspaces is reduced through a scalable manifold clustering objective based on l1-minimization. Insight into the number and corresponding dimensionality of these physical regimes is gained as a byproduct of this clustering method. Additionally, while the sparsity inherent in the dual snapshots causes them to appear artificially high-dimensional when considering their singular value spectrum, it is not the case that a large number of degrees of freedom is required to accurately represent the associated contact forces. Nonnegative matrix completion techniques are used to efficiently compress the sparse dual snapshots into a suitable subspace for the resulting dual ROB. The performance of this framework is assessed for several nonlinear contact problems. [1] M. Balajewicz, D. Amsallem and C. Farhat, Projection-Based Model Reduction for Contact Problems, International Journal for Numerical Methods in Engineering, Vol. 106, pp. 644-663 (2016) [3] C. Farhat, T. Chapman and P. Avery, Structure-Preserving, Stability, and Accuracy Properties of the Energy-Conserving Sampling and Weighting (ECSW) Method for the Hyper Reduction of Nonlinear Finite Element Dynamic Models, International Journal for Numerical Methods in Engineering, Vol. 102, pp. 1077-1110 (2015) [2] D. Amsallem, M. Zahr and C. Farhat, Nonlinear Model Order Reduction Based on Local Reduced-Order Bases, International Journal for Numerical Methods in Engineering, Vol. 92, pp. 891-916 (2012)

14th U.S. National Congress on Computational Mechanics
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Title: Density Estimation for a Class of Elliptic Problems on Stochastically Perturbed Domains

Author(s): *Jehanzeb Chaudhry, *University of New Mexico*; Donald Estep, *Colorado State University*; Nathanial Burch, *Gonzaga University*.

We study elliptic partial differential equation boundary value problems for which the domain where the equations are posed is uncertain. In order to model this uncertainty, we formulate a class of problems that are posed on stochastic domains. Of particular interest is the nonparametric density estimation problem for a quantity of interest. We introduce a piecewise transformation of the domain to a deterministic reference domain and exploit for efficiency the transformation in a Monte Carlo sampling procedure so that many samples can be obtained to approximate the distribution at a reasonable cost. We present an a posteriori error analysis for each sample and for the empirical distribution function obtained from the samples, which reflect the various deterministic and statistical sources of error.

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Title: Effect of Lipid Type and Surface Charges on the Bending Modulus of Lipid Bilayer Membranes

Author(s): *Adarsh Chaurasia, Andrew Rukangu, Eric Freeman, *University of Georgia*; Michael Philen, Gary Seidel, *Virginia Tech*.

Lipid bilayers form an important part of all living cells and help with regulation of cellular activity through the cell wall. These phospholipids have a hydrophilic head and a hydrophobic tail, which in an aqueous environment results in self-assembly into bilayers with two layers of lipids across the membrane. The bilayer bending modulus is considered to play a key role in determining the cellular function e.g. endocytosis and exocytosis. The current work aims to computationally explore the bilayer bending modulus for different lipid types associated with the cellular fusion mechanism, specifically in terms of the effect of surface charges on the lipid head groups. Traditionally, the bending modulus has been evaluated computationally using molecular dynamics (MD) simulations to model the membranes and analyzing the thermal undulations of the interface through the power spectra of these undulations. Some recent studies have shown that the undulation power spectra under predicts the bilayer bending modulus as compared to experimentally reported values. An alternative approach based on the power spectra of lipid orientations in the membrane has been proposed in recent literature. In the current work, the bilayers are modeled using coarse grained (CG) MD simulation using the MARTINI force field. The extracted CG MD data is analyzed using Fourier transforms of the undulations and orientation vectors to establish the differences between the two approaches. Several other simulation parameters (e.g. bilayer size, simulation time) are systematically studied to understand their effect on the estimated bilayer bending modulus and to establish convergence in results. Finally, a parametric study is conducted to evaluate the bilayer bending modulus for a set of lipids associated with the cellular fusion process. Additionally, the effect of surface charge in the lipid head group is evaluated with varying salt concentration in the aqueous solution which has been observed to affect the resulting bending modulus. The computational results obtained are validated against experimentally observed bending modulus obtained using the undulation spectra of spherical vesicles created using electroformation for a subset of lipid types. The surface contours are extracted using image analysis tools form high speed videos to study the thermal undulations. The computational results obtained from the orientation spectra are observed to predict the experimentally estimated bending moduli. The results obtained from the study are expected to provide insight into the biophysical nature of cellular mechanisms in terms of surface interactions between different living and model cells.

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Title: A Cell-Centered Method for Solving 2D-Axisymmetric Updated Lagrangian Hyper-Elastoplasticity Equations

Author(s): *Rémi Chauvin, Isabelle Bertron, Pierre-Henri Maire, *CEA/CESTA, Le Barp, France*; Patrick Le Tallec, *Ecole Polytechnique, Palaiseau, France*.

Summary of the presentation: we present herein a cell-centered method for solving the hyper-elastoplasticity equations written under updated Lagrangian formalism for both bidimensional and 2D-axisymmetric problems. The method is entropic and conservative for the sake of capturing intense shock waves. The numerical modeling of fast transient dynamics phenomena characterized by large deformations and high strain rates is a topic of great interest for industrial applications such as high velocity impacts. Nowadays, the development of Finite Volume discretization for Lagrangian solid dynamics seems to be a promising alternative to the traditional Finite Element approaches in particular for simulating very fast dynamic phenomena involving shock waves [1]. Furthermore, the utilization of an hyper-elastic [2] model instead of the so-called Wilkins hypo-elastic model presents both theoretical and numerical advantages since it is naturally objective, conservative and thermodynamically consistent. In this work we deal with isotropic hyper-elastoplastic model in which von Mises yield criterion is used. A bidimensional finite volume discretization of equations written under updated Lagrangian formalism is presented. A cell-centered formulation in which the fluxes are defined at nodes for the sake of naturally satisfying the Geometric Conservation Law is presented. The subcell force expression in terms of the cell-centered stress tensor, the nodal velocity and the cell-centered velocity have been derived to enforce a local entropy inequality at the semi-discrete level ensuring the conversion of kinetic energy into internal energy through irreversible processes such as shock waves. We also note that this discretization guaranties the conservation of total energy and momentum. The second-order time and space discretization is obtained by means of an acoustic Generalized Riemann Problem (GRP) approach. An extension of the method to axisymmetric problems using a control volume formulation is developed in order to perform realistic high velocity impact simulations. Academic validations and experimental comparisons using both hyper-elastoplastic model and Wilkins model are shown to point out the relevancy of the approach. [1] Lee C. H., Gil A. J. and Bonet J.: Development of a cell centered upwind finite volume algorithm for a new conservation law formulation in structural dynamics" Computers and Structures, 2013. [2] Gurtin M.E., Fried E., Anand L.:The Mechanics and Thermodynamics of Continua. Cambridge University Press, 2009. [3] Maire P.-H., Abgrall R., Breil J., Loubère R., Rebourcet B.: A nominally second-order cell-centered Lagrangian scheme for simulating elastic-plastic flows on two-dimensional unstructured grids. Journal of Computational Physics 235:626-665, 2013.

14th U.S. National Congress on Computational Mechanics
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Title: An Anisotropic Distribution Dislocation Loop Model for Simulation of Nanoindentation of Single Crystals

Author(s): *Y. P. Chen, *Huazhong University of Science*.

An anisotropic distribution dislocation loop model is proposed for simulation of nanoindentation of single crystals based on the recently available solution of the elastic displacement and stress fields due to a polygonal dislocation within an anisotropic homogeneous half-space [1]. The present investigation is a direct extension of the approach established by Mura et al. [2], and its recent application to triangular dislocation loop model [3], which is only capable of describing the indentation processes of isotropic materials, thus ruling out the possibility of characterizing the nanoindentation of elastically anisotropic single crystals. By following the procedure of Mura et al. [2], we adopt square and triangular prismatic dislocation loops as building blocks with Burgers vectors normal to the free surface to simulate the Vickers and Berkovich indentation, respectively. However, we place all the prismatic dislocation loops (PDLs) within a semi-ellipsoidal volume rather than a semi-spherical region as adopted by Mura et al. [2] after analysing the existing simulation results based on dislocation density formulation (Huang et al., 2000). The nanoindentation is performed in [001] and [111] crystallographic directions employing Vickers and Berkovich indentors, respectively, and different magnitude of pile-up, sink-in and spring-back is observed in different directions, clearly demonstrating the effects of elastic anisotropy of the indented single crystals on nanoindentation, hence a further improvement of the original model of Mura et al. [2]. Keywords: nanoindentation, anisotropic prismatic dislocation loop, pile-up and sink-in. Acknowledgement: The project is supported by National Natural Science Foundation of China NSFC (11272129). References: [1] Chu, H. J., Pan, E., Wang, J., Beyerlein, I. J., 2012. Elastic displacement and stress fields induced by a dislocation of polygonal shape in an anisotropic elastic half-space. Journal of Applied Mechanics 79, 021011-1-021011-9. [2] Mura, T. ,Yamashita, N., Mishima, T., Hirose, Y., 1989. A dislocation model for hardness indentation problems. Int. J. Engng Sci. 27(1), 1-9. [3] Muraishi, S., 2013. Triangular dislocation loop model for indented material. Mechanics of Materials 56, 106-121.

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Title: Recent Advances in Improving the Spatial and Temporal Discretization Schemes of the Material Point Method for Better Simulating Transient Responses

Author(s): *Zhen Chen, *DLUT / MU*; Yong Gan, *Zhejiang University*; Yonggang Zheng, *Dalian Univ. Technology*.

To simulate multiphase (solid-fluid-gas) interactions involving failure evolution without invoking a master/slave nodal treatment at the contact surface, the material point method (MPM) has evolved over the last two decades, and been applied to many areas in simulation-based engineering science, as shown in the recent comprehensive literature survey [1]. Recent research focus has been on multiscale and multiphysics simulation of structural responses to transient loading [2 and 3, among others]. To eliminate the effect of the cell-crossing error on numerical solutions obtained with the original MPM, much research has been performed by many researchers in the recent years [1]. In this talk, we will present our recent research results in improving the spatial and temporal discretization schemes of the MPM for better simulating transient responses, in which the mapping and remapping process in space is enhanced with B-spline basis functions, and the displacement and velocity fields in a time interval are interpolated with the piecewise cubic and linear functions, respectively. Future research directions will be discussed based on the current findings. References: [1] Zhang, X., Chen, Z., and Liu, Y., The Material Point Method – A Continuum-Based Particle Method for Extreme Loading Cases, Elsevier, 2016. [2] Jiang, S., Chen, Z., Sewell, T.D., and Gan, Y., “Multiscale Simulation of the Responses of Discrete Nanostructures to Extreme Loading Conditions Based on the Material Point Method,” Computer Methods in Applied Mechanics and Engineering, Vol. 297, pp. 219-238, 2015. [3] Tao, J., Zheng, Y.G., Chen, Z., and Zhang, H.W., “Generalized interpolation material point method for coupled thermo-mechanical processes,” International Journal of Mechanics and Materials in Design, Vol. 12, pp. 577-595, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: Intrinsic Cohesive Modeling of the Impact Cracking of Laminated Glass

Author(s): *Shunhua Chen, Shinobu Yoshimura, Tomonori Yamada, *The University of Tokyo*.

In recent years, a growing interest has been devoted to investigating the impact cracking of laminated glass plates by means of numerical and experimental approaches. However, the impact cracking mechanism of a laminated glass plate has not been thoroughly explained. The purpose of this work is to numerically investigate the impact cracking mechanism of the laminated glass plate in the framework of intrinsic cohesive modeling. The impact cracking behaviors of a laminated glass plate are simulated, and the simulation results are validated by comparison with the corresponding experimental ones. Parametric studies are performed to investigate the influence factors of crack onset and propagation in the laminated glass plate.

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Title: Adaptive Refinement of Hierarchical T-Splines

Author(s): *Lin Chen, René de Borst, *University of Sheffield*.

Adaptive splines have been studied as an effective tool for local refinement in isogeometric analysis (IGA). In IGA, the NURBS basis functions from the computer aided design (CAD) model are directly employed in the computational model. The approximation error from geometry description is alleviated, comparing to the standard finite element method. However, due to the tensor product structure of NURBS, finer grids are difficult to achieve without the propagation of the refinement. Ideally, the IGA should be combined with locally adaptive mesh refinement to provide a finer mesh with the exact geometry representation preserved. Various local refinement strategies have been developed recently, including T-splines, hierarchical and truncated hierarchical B-splines [1]. T-splines were introduced by Sederberg. Then, they have been introduced in IGA by Bazilevs and implemented in the Bèzier extraction framework by Scott et al. [1]. Recently, the local refinement of T-splines has been investigated [1, 2], which enriches their abilities. The hierarchical refinement of T-splines and truncated hierarchical T-splines combines the local refinement abilities of hierarchical B-splines with the geometrical representation capabilities of T-splines. The basic idea is to locally enrich the approximation space by replacing selected coarse grid T-splines with fine grid T-splines. In this contribution, we present an adaptive local refinement technique for IGA based on hierarchical T-splines. The properties of hierarchical T-splines are investigated, e.g. the nested nature, the linear independence and the partition of unity. An element-wise viewpoint is adopted for implementation, which facilitates the application of Bèzier extraction and adaptive refinement in the analysis. In the implementation, a multi-level T-spline mesh is constructed by successive cell subdivisions of an initial coarse T-spline mesh. Then, on each hierarchy level, Bèzier extraction is applied to obtain the stiffness matrix without consideration of the multi-level interaction. The interaction is recovered by the subdivision operator. Numerical examples are presented to demonstrate the accuracy of the method. Promising results are obtained. [1] Evans, E., Scott, M., Li, X., Thomas, D. (2015). Hierarchical T-splines: Analysis-suitability, Bézier extraction, and application as an adaptive basis for isogeometric analysis. Computer Methods in Applied Mechanics and Engineering, 284, 1-20. [2] Wei, X., Zhang, Y., Liu, L., Hughes, T. (2016). Truncated T-splines: Fundamentals and methods. Computer Methods in Applied Mechanics and Engineering, 316, 349-372.

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Title: Computational Design and Additive Manufacturing of Periodic Conformal Metasurfaces by Synthesizing Topology Optimization with Conformal Mapping

Author(s): *Shikui Chen, Panagiotis Vogiatzis, *SUNY Stony Brook University* ; Ming Ma, Xianfeng David Gu, *SUNY Stony Brook University*.

Conformal metasurfaces have wide applications in different areas, including conformal cooling structures, orthopedic and prosthetic devices, and self-supporting surface structures. In this paper, we present a computational approach for systematic design and integrated additive manufacturing of spatial free-form periodic metasurfaces. The proposed scheme rests on the level-set based topology approach and the conformal mapping theory. A 2D unit cell of metamaterial with tailored effective properties is created using the level-set based topology optimization method. The achieved unit cell is further mapped to the 3D quad meshes on a free-form surface by applying the conformal mapping method which can preserve the local shape and angle when mapping the 2D design to a 3D surface. The proposed level-set-based optimization methods not only can act as a motivator for design synthesis but also can be seamlessly hooked with additive manufacturing with no need of CAD reconstructions. The proposed computational framework provides a solution to increasing applications involving innovative metamaterial designs on free-form surfaces in different fields of interest. The performance of the proposed scheme is illustrated through a benchmark example where a negative-Poisson's-ratio unit cell pattern is mapped to a 3D human face and fabricated through additive manufacturing.

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Title: Finite Element Modeling of Ceramic Deposition by LBM (SLM) Additive Manufacturing

Author(s): *Qiang Chen, Gildas Guillemot, Charles-André Gandin, Michel Bellet, *Mines ParisTech*.

In the last decade, Additive Manufacturing (AM) has been largely developed and considered as the symbol of the next industrial revolution. Among AM techniques, Laser Beam Melting (LBM) or Selective Laser Melting (SLM) is able to produce parts with good mechanical properties. However, efficient production remains challenging as the links between structures and processing parameters are not sufficiently understood and mastered, especially for ceramic materials. Thus, a numerical model is proposed to investigate the complex phenomena occurring at the scale of track formation, including the laser material interaction, the flow dynamics in the melt pool and the stresses build-up after solidification. This 3D numerical model uses a Level Set (LS) Finite Element formulation to capture the boundary between the gas and material domain, with application to alumina*. Considering the weak absorption of the Nd:YAG laser radiation by alumina, a volumetric heat source model based on the Beer-Lambert law is developed. With the LS formulation, properties are averaged at the boundary between the present domains as a function of the local fraction of phases and their intrinsic temperature-dependent properties. A compressible Newtonian behavior is introduced to model the condensation from powder to dense matter. The dynamics of melt pool is modeled considering the surface tension and Marangoni effects. A mesh adaptation is used to track the evolving surface of the melt pool. In addition to the previous thermal-hydraulic calculation, a second resolution is performed at each time increment in order to describe local strains and associated stresses, using an elasto-visco-plastic behavior law in the consolidated material. Several simulations demonstrate the influence of the laser velocity and power, as well as the powder layer thickness on temperature field and track shape. The dynamics of melt pool and its influence on temperature distribution and track shape are investigated by different values of the viscosity, the surface tension coefficient and its dependence on temperature. The stresses build-up during the deposition process is presented. The effect of preheating is studied by adding a second laser source. At last, multiple passes with different scanning strategies are compared. From a practical viewpoint, this study should help to optimize process parameters to offer a better control of the track shape and avoid potential cracks. * Q. Chen, G. Guillemot, Ch.-A. Gandin, M. Bellet, Three-dimensional finite element thermomechanical modeling of additive manufacturing by selective laser melting for ceramic materials, Additive Manufacturing, in press.

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Title: An Intermediate Homogenization Approach for Peridynamic Modeling of Failure in Heterogeneous Materials

Author(s): *Ziguang Chen, Sina Niazi, Florin Bobaru, *University of Nebraska-Lincoln*.

The peridynamic (PD) theory, introduced by Dr. Stewart Silling [1] as a reformulation of the classical continuum mechanics, is an integral-type nonlocal model that allows fracture and damage to be treated as natural parts of the solution process. In PD theory, the interaction between a material point and its neighbors extends beyond the nearest neighbors, over a region called “the horizon”. Within this non-local region, small scale heterogeneities, such as multiphase distribution and material defects, can be represented by the variation of the mechanical bonds. We introduce a new Intermediate Homogenization approach (IH-PD model) for failure in multiphase materials. Different from the Locally-Homogenized approach (LH-PD model, reported in [2]), in which the bond properties are computed locally based on an equivalent homogenized composite material, in the IH-PD model we have two types of bonds, inter-phase and intra-phase bonds, which represent the properties of the distinct composite phases and of interfaces between them. For example, for a two-phase composite with phases A and B, we define A-A bonds (inter-phase), A-B bonds (intra-phase), and B-B bonds (inter-phase). The distribution of the different bonds depends on the volume fraction of the phases in the nodes. While the specific geometry of the microstructure is not preserved, the specific volume fraction is and, in many instances, this is critical in modeling evolution of fracture and damage. We observe that the difference in results between the LH-PD and IH-PD models for problems in which extreme dynamics controls the crack behavior is small. However, for problems in which the microstructure dictates the critical phenomenon, the IH-PD model is able to capture an evolution of the failure not seen with the LH-PD model. Indeed, when a porous material (two-phase composite in which one of the phases is void) is considered under quasi-static loading, the IH-PD model reproduces the experimentally observed dependence of crack initiation and growth on the size of a pre-notch, while the LH-PD model, due to ignoring of any microstructural details, fails to do so. We find that the IH model is as computationally efficient compared with the LH model, which lead us to recommend it for modeling failure in composite and/or porous materials. References [1] Silling S.A., J. Mech. Phys. Solids, 48 (2000) 175-209. [2] Cheng Z, Zhang G, Wang Y, Bobaru, F., Composites and Structures, 133: 529-546, (2015).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Reproducing Kernel Particle Method Framework for Modeling Failure of Solids Subjected to Blast Loadings

Author(s): *J. S. Chen, *University of California, San Diego*; Guohua Zhou, Mike Hillman, *The Pennsylvania State University*.

The numerical simulation of transient dynamic failure of structures subjected to blast loadings requires the key physics such as strong shocks in fluid (explosive gas and air) and solid media, fluid-structure interaction, material damage and fragmentations, and multi-body contact to be properly considered in the mathematical formulation and the associated numerical algorithms. These dominant phenomena in blast events yield “rough solution” in the conservation equations in the form of moving discontinuities that cannot be effectively modeled by the conventional finite element methods. A semi-Lagrangian meshfree Reproducing Kernel Particle Method (RKPM) framework [1] is proposed to model such extreme events in this study. In this work, shock waves in both air and solid are modeled by embedding the Godunov flux into the semi-Lagrangian RKPM formulation in a unified manner. The essential shock physics are introduced in the proposed node-based Riemann solver, and the Gibbs oscillation is limited by introducing a gradient smoothing technique [2, 3]. In this thesis, two formulations are proposed and verified by solving a set of multi-dimensional benchmark problems involving strong shocks in fluids and solids. The air-structure interface is treated by a level set enhanced natural kernel contact algorithm [4], which does not require the definition of potential contact surfaces a priori. The blast-induced fragmentation is simulated by the damage model under the semi-Lagrangian RKPM discretization without using the artificial element erosion technique. Several benchmark problems have been solved to verify the accuracy and performance of the proposed numerical formulation. This computational framework is then applied to the simulation of a reinforced concrete column subjected to blast loading and explosive welding processes, demonstrating the effectiveness and robustness of the proposed methods. References [1] Guan, C., Chi, S. W., Chen, J. S., Slawson, T. R., Roth, M. J., “Semi-Lagrangian Reproducing Kernel Particle Method for Fragment-Impact Problems,” International Journal of Impact Engineering, Vol. 38, 1033-1047, 2011. [2] Roth, M. J., Chen, J. S., Slawson, T. R., Danielson, K. D., “Stable and Flux-Conserved Meshfree Formulation to Model Shocks,” Computational Mechanics, Vol. 57, pp. 773–792, 2016. [3] Roth, M. J., Chen, J. S., Danielson, K. D., Slawson, T. R., “Hydrodynamic Meshfree Method for High-Rate Solid Dynamics using a Rankine-Hugoniot Enhancement in a Riemann-SCNI Framework”, International Journal for Numerical Methods in Engineering, DOI: 10.1002/nme.5266, 2016. [4] Chi, S. W., Lee, C. H., Chen, J. S., Guan, P. C., “A Level Set Enhanced Natural Kernel Contact Algorithm for Impact and Penetration Modeling,” International Journal for Numerical Methods in Engineering, Vol. 102, pp. 839–866, 2015.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Dynamic Multiscale Method and Applications

Author(s): *Chuin-Shan David CHEN, *National Taiwan University*.

Atomistic-based multiscale modeling theory and computational method for static problems have been successfully developed in the past decade. The advance has transformed the way we design micro and nanoscale materials for static problems. In contrast, the development of dynamic multiscale method for non-equilibrium simulations is limited due to spurious wave-reflection problems on the interface between atoms and continuum. In this talk, I will present our recent work on developing a generalized absorbing boundary condition for arbitrary geometries and a novel multiscale non-equilibrium simulations based on this concept. In the first part of my talk, I will present a semi-analytical solution of time history kernel for a generalized absorbing boundary condition. The concept of virtual atoms in real space that can conform with an arbitrary boundary in an arbitrary lattice is adopted to facilitate the kernel derivation. The generalized Langevin equation is regularized by eigenvalue decomposition and consequently an analytical expression of an inverse Laplace transform is obtained. Together with a careful construction of dynamical matrix in the virtual domain, a semi-analytical form of the time history kernel functions for an arbitrary boundary in an arbitrary lattice can be found. The treatment not only significantly reduces computational cost but also releases the planar boundary restriction when the kernel is computed in the frequency domain. The time history kernel functions for different crystal lattices are derived to show the generality of the proposed method. The concept of finite-size virtual domain furthermore allows us to construct a novel dynamic multiscale modeling method for non-equilibrium simulations. Dynamic responses of atoms in the virtual domain can now be effectively constructed through a careful choice of time history kernels. In the second part of my talk, I will present a novel dynamic multiscale modeling method based on the generalized absorbing interface. The proposed method allows us to overcome length scale limitation posed on non-equilibrium molecular dynamics (NEMD) simulations. Applications of the dynamic multiscale method for thermal transport simulations will be addressed.

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Title: Biomechanical Models for Early Embryonic Brain Morphogenesis

Author(s): Hannah Grover, Wei Zheng, Shicheng Huang, Yan Li, Nan Hu, *Zi Chen, *Dartmouth College*; Lina Zang, *Shanghai Jiao Tong University*.

The proper development of the neural tube (NT) is essential to embryonic morphogenesis(1). When the NT does not form properly, abnormalities in brain development known as neural tube defects (NTDs) can occur(1-3). Flexure and torsion of the developing NT are two of the early events in morphogenesis that lead to left-right asymmetry in embryos. The biomechanical mechanisms underlying this left-right asymmetry are not fully understood(1,3). Computational modeling is now becoming more prevalent in biology to aid in modelling these complex events. The goal of our research is to determine the role of mechanical forces in NT morphogenesis. We employ computational modeling to further elucidate the mechanical forces involved in NT morphogenesis. Our research is focused on the early brain development of the chick embryo, which is a popular model for human embryonic morphogenesis due to the similarity in development. In chick embryos, flexure and torsion of the NT change from Hamburger Hamilton (HH) stage 12 to 17(1). There are multiple potential driving factors behind flexure and torsion which we hope to either eliminate or verify in our hypotheses(1). To quantify the flexure and torsion of the NT, optical coherence tomography (OCT) imaging is used. OCT is a non-invasive and non-destructive imaging method which generates 2D cross-sectional and 3D volumetric images of live embryos. OCT imaging was performed from HH12-HH17 to build a control model for computational simulations. To aid in interpreting our experimental results, a 3D finite-element model of an embryo during HH14-17 was constructed using the commercial finite element software, Abaqus. The results of the research so far indicate that: 1) The cranial and thoracic curvatures both change while the cervical curvature remains mostly unchanged during growth and 2) simulations show that the radius ratio between different flexures and the aspect ratio of the brain cross-section affect torsion. This is significant as the previous model, which used estimates and a combined cranial/cervical curvature, may not accurately reflect the changes in radius of curvature that occurs during embryonic growth. In the future, modeling of these earlier embryonic stages may prove beneficial to further understanding the process of normal growth and development, as well as the formation of congenital defects. [1] Chen, Z. et al (2016). ■J. R. Soc. Interface, 13(124). [2] Greene, N. D. E., & Copp, A. J. (2009). Prenatal Diagnosis, 29(4), 303–311. [3] Wyczalkowski, M. A. et al. (2012). Birth Defects Res C , 96(2), 132–152.

14th U.S. National Congress on Computational Mechanics
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Title: Lattice Topology Optimization with Design-Dependent Feature Evolution for Heat Conduction Problem

Author(s): *Lin Cheng, Albert Chi Fu To, *University of Pittsburgh*.

Additive manufacturing holds great promise to be the revolutionary technique due to its capability to economically fabricate complex geometry, such as porous lattice structure, which is lightweight and high-performing. Hence, lattice infill topology optimization recently has drawn remarkable interest and a variety of methods have been developed to promote the research of lattice design. On the other hand, lattice infill cannot be span to functional features with firm geometric form, widely existing in thermal products, like holes and cooling channels. To fill this gap, a concurrent topology optimization is proposed to combine the feature evolution into the lattice topology optimization, which can optimize the lattice layout and feature parameters simultaneously. In particular, the movable features subject to design-dependent boundary conditions, like heat flux and heat convection, are schematically studied. And parametric level set functions and R-functions are employed for the representation of the features and attached boundaries. They are then implemented into the material interpolation for finite element analysis (FEA) and sensitivities calculation for both lattice structure and movable features, in order to solve the problem through a unified gradient based approach. Several numerical examples are provided to demonstrate the efficiency and robustness of proposed method. More importantly, we emphasize the 3D study with practical application instead of simple two-dimensional (2D) model, and the comparison between the optimal results and full scale simulation shows great agreement.

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Title: Numerical Simulations of In-Stent Restenosis

Author(s): *Jie Cheng, Lucy Zhang, *Rensselaer Polytechnic Inst*.

The in-stent restenosis is a common adverse event of endovascular procedures. It pertains to stenting treatment for arteries or blood vessels that have become narrowed, and subsequently become re-narrowed as a result of the stent placement. In this talk, we predict the restenosis through simulations by implementing a stress-modulated growth model using the multiplicative decomposition approach in finite elements. Based on the growth model, the impact of the stent design on the restenosis rate of an in-stent coronary artery is investigated. A strong correlation between the stent shape and restenosis rate due to the stress distribution on the artery wall is found. The results indicate that careful stent designs can reduce stress concentration, thereby reduce the rate of restenosis. It is also demonstrated in this study that soft tissue growth models can facilitate more effective designs of medical devices.

14th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Process-to-Structure Heuristics for Additively Manufactured Materials

Author(s): *Puikei Cheng, Wing Kam Liu, *Northwestern University*.

Laser Engineered Net Shaping (LENS) is a flexible additive manufacturing (AM) process that deposits and fuses metal powder directly onto a 3D substrate. While versatile, the LENS process is extremely localized and results in inhomogeneous microstructures. There is a high levels of anisotropy within builds as well as low repeatability between similar builds, both which render LENS materials unsuitable for mission-critical applications. One proposed solution is to perform online monitoring of the part during the build and tune process parameters in situ to achieve improved bulk properties. To do so, we can try to relate the resulting microstructures to the thermal history of each point in the build. However, this is challenging due to the high number of process parameters involved in the LENS process. Additionally, there must be enough microstructural data to resolve the effects of varying process parameters. To remedy this, we first obtained several LENS builds with full toolpath and IR information. We then developed a testing procedure to extract as much spatially-varying microstructural information as possible. With an in-house thermal finite element model, we can then correlate point-by-point the microstructure to thermal histories obtained via simulation. Determining correlations between process and microstructure variables will allow for focused experiments targeting specific parameter relationships and the advancement of relevant physics-based models.

14th U.S. National Congress on Computational Mechanics
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Title: On the Mixed Virtual Element Method (VEM) for Finite Deformations

Author(s): *Heng Chi, Glaucio Paulino, *Georgia Institute Technology*; Lourenco Beirao da Veiga, *University of Milano-Bicocca*.

The virtual element method (VEM), based on mimetic technology, is extended to finite deformations in the present work. Specifically, we present a projection-based VEM framework for finite elasticity considering a two-field mixed formulation, which emphasizes two issues: stabilization and element-level volume change (volume average of the determinant of the deformation gradient). To address the former issue, we introduce a novel stabilization scheme that evolves with the deformation level, which better captures highly heterogeneous and localized deformations. For the later issue, we provide exact evaluations of the average volume change in both 2D and 3D on properly constructed local displacement spaces. Convergence and accuracy of the proposed mixed VEM are verified by means of numerical examples using unique element shapes inspired by Escher (the artist), and an engineering application is demonstrated.

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Title: High Order Gradient Reproducing Kernel Collocation Method for High Order PDEs

Author(s): *Sheng-Wei Chi, Ashkan Mahdavi, *Univ. of Illinois at Chicago*.

The Reproducing Kernel approximation in conjunction with the Collocation Method (RKCM) [1] was introduced for solutions of PDEs and engineering problems some time ago. Although it offers only algebraic convergence, being less sensitive to the nodal distribution and of compact structure, thus better conditioning, make it an attractive method for engineering applications. However, taking direct derivatives of the reproducing kernel approximation is computationally expensive, in comparison to other commonly used approximations for collocation methods, such as RBFs. In this work, we address the high computational cost in the RKCM while achieving optimal convergence by adopting gradient reproduction kernel approximations for all derivatives involved in a PDE. In contrast to the earlier work in [2], both first order and second order derivatives involved in the approximation for a second order PDE are expressed by gradient reproducing kernels in the present method. We show that the same number of collocation points and source points can be used in the HG-RKCM for optimal convergence. The present method is further introduced for problems governed by 4th order PDEs, such as Kirchhoff plate problems and 4th order phase-field model for fracture [3]. The numerical studies show that the present method is much faster and more robust than the RKCM. References: [1] H. Y. Hu, J. S. Chen, and W. Hu, Weighted radial basis collocation method for boundary value problems, International Journal for Numerical Methods in Engineering 69, p.2736-2757, 2007. [2] S.W. Chi, J.S. Chen, H.Y. Hu, and J.P. Yang, A gradient reproducing kernel collocation method for boundary value problems, International Journal for Numerical Methods in Engineering 93(13), p.1381-1402, 2013. [3] M.J. Borden, T. J.R. Hughes, C. M. Landis, C. V. Verhoosel, A Higher-Order Phase-Field Model for Brittle Fracture: Formulation and Analysis within the Isogeometric Analysis framework, Computer Methods in Applied Mechanics and Engineering, 273, p. 100-118, 2014.

14th U.S. National Congress on Computational Mechanics
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Title: Mapped Finite Element Methods: Higher Order Solutions of Problems with Singularities

Author(s): *Maurizio M. Chiaramonte, *Princeton University*.

High order finite element solutions of crack an re-entrant corner problems in elasticity are noto- riously challenging to attain. The slow convergence rates for these classes of problems are tied to the low degree of regularity possessed by the solution. The need for high order solutions is motivated by long running simulations of crack propagation. In fact, as the error in the crack path grows non- linearly, it is of uttermost importance to accurately resolve the elasticity fields at each time step. The above ensures that the final computed crack paths are within reasonable tolerance of the exact one without excessive computational expenditures. To this extent, we develop higher order finite element methods for crack and re-entrant corner problems in elasticity. The method [1] exploits the a priori knowledge of the singular behavior of the fields to construct an alternate regular solution. Solving for the alternate problem yields optimal rates of convergence and high order of accuracy. Namely, standard finite element error estimates in the L2 and H1 norm are proved to hold, both for the alternate solution and the composed alternate solution. The salient feature of the method is the lack of additional degrees of freedom in comparison with standard Galerkin finite element formulation. Effectively, for the same computational cost we obtain a higher order of accuracy. Furthermore, unlike other state of the art tools, the method preserves the well conditioned nature of the system of equations and does not require the knowledge of the exact asymptotic behavior, hence the method can be readily applied to singular problems for which we are not endowed with an explicit asymptotic solution such as cracks in graded materials. The method is verified with respect several analytical solutions in two- and three-dimensions accounting for the possible curvilinear (non-planar) geometry of cracks as well as material inhomogeneities. References: [1] Maurizio M. Chiaramonte, Yongxing Shen, and Adrian J. Lew. Mapped finite element methods: High-order approximations of problems on domains with cracks and corners. International Journal for Numerical Methods in Engineering, 2017.

14th U.S. National Congress on Computational Mechanics
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Title: Cohesive Polygonal Finite Elements for Modeling Pervasive Fracture

Author(s): *Eric B. Chin, N. Sukumar, *UC Davis*; Joe Bishop, *Sandia National Laboratories*; Rao Garimella, *Los Alamos National Laboratory*.

We introduce a framework for modeling dynamic fracture problems using cohesive polygonal finite elements. This framework is designed to easily extend to three-dimensional problems using polyhedral finite elements – the focus of related future work. Dynamic fracture is pervasive in the sense that a multitude of cracks can nucleate, coalesce, branch, and propagate in arbitrary directions. Random polygonal meshes provide a robust, efficient method for generating an unbiased network of fracture surfaces. Further, these meshes have more facets per element than standard triangle or quadrilateral meshes, providing more possible surfaces to insert cohesive surfaces. For these reasons, polygonal meshes have been shown to be a good fit for capturing pervasive fracture [1]. We use both Wachspress and maximum entropy basis functions to form a finite element basis over the polygons. Fracture surfaces are captured through dynamically inserted cohesive zone elements at facets between the polygons in the mesh. As the analysis progresses, we track and update the evolving mesh topology using Mesh Toolkit (MSTK) [2], a flexible library that allows for querying and manipulating unstructured polygonal and polyhedral meshes. Contact is enforced through a penalty method which is applied to both closed cohesive surfaces and general interpenetration of two polygonal elements. Several numerical examples are presented which illustrate the capabilities of the method and demonstrate convergence of solutions. References: [1] Bishop J.E. “Simulating the pervasive fracture of materials and structures using randomly close packed Voronoi tessellations,” Computational Mechanics, vol. 44, pp. 455—471, 2009. [2] Garimella R.V. “MSTK - A Flexible Infrastructure Library for Developing Mesh Based Applications,” Proceedings of the 13th International Meshing Roundtable, pp. 203—212, 2004 (https://github.com/losalamos/MSTK).

14th U.S. National Congress on Computational Mechanics
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Title: Discontinuous Galerkin Method for Predicting Heat Transfer in Hypersonic Environments

Author(s): *Eric Ching, Yu Lv, Matthias Ihme, *Stanford University*.

Hypersonic stagnation heating results computed with conventional finite-volume techniques deteriorate significantly on unstructured grids, particularly those without shock alignment [1]. This often limits finite-volume schemes to structured grids, which lack the geometric flexibility commonly needed for hypersonic applications and can require considerable user intervention to adapt the grid to strong shocks. Furthermore, finite-volume schemes have been shown to be very sensitive to the inviscid flux function, limiters, and other factors [2]. One promising approach to obtaining robust heat transfer predictions is high-order methods [3]. This study discusses the development of a robust shock capturing methodology for high-order discontinuous Galerkin schemes. Shocks are detected based on pressure jumps and stabilized using a smooth artificial viscosity formulation. To minimize parametric dependence, an optimization method is formulated that results in the least amount of artificial viscosity necessary to sufficiently suppress nonlinear instabilities and achieve steady-state convergence. The performance of this method is evaluated in fourth-order-accurate computations of hypersonic flows over a circular half-cylinder and a double cone. The former test case is a simple configuration, useful for exposing algorithmic deficiencies, while the latter represents a significantly more challenging flow with strict resolution requirements and complex shock interactions. Compared to finite-volume methods, results show this methodology to be significantly less sensitive to mesh topology and the inviscid flux function. [1] Gnoffo, P. A. and White, J. A., Computational aerothermodynamic simulation issues on unstructured grids, 37th AIAA Thermophysics Conference, Portland, OR, AIAA Paper 2004-2371, Jun. 2004. [2] Kitamura, K., A further survey of shock capturing methods on hypersonic heating issues, 21st AIAA Computational Fluid Dynamics Conference, San Diego, CA, AIAA Paper 2013-2698, Jun. 2013. [3] Barter, G. E. and Darmofal, D. L., Shock capturing with PDE-based artificial viscosity for DGFEM: Part I. Formulation, Journal of Computational Physics, Vol. 229, No. 5, 2010, pp. 1810-1827.

14th U.S. National Congress on Computational Mechanics
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Title: Multiscale Computational Homogenization Approach of Polymer Nanocomposites Including the Clustered Nanoparticles

Author(s): *Maenghyo Cho, Hyunseong Shin, Kyungmin Baek, Jin-Gyu Han, *Seoul National University*.

In spite of rapid development of fabrication technique, non-uniform dispersion of the reinforced nanoparticles is still inevitable. Non-uniformly distributed nanoparticles due to high non-bond interaction such as van der Waals interaction and electrostatic forces form the cluster of nanoparticles. The molecular dynamics simulation results indicated that the elastic properties of interphase zone decrease as the interparticulate distance decreases due to the weak formation of interphase zone near nanoparticles. Due to insufficient permeation of molecular chain of host thermoplastic materials into the gallery zone of nanoparticles, the agglomeration of nanoparticles plays a role of a vacancy defect inside the interphase zone. We develop the interphase percolation model to reflect this molecular phenomenon near the agglomerated nanoparticles. The multiscale homogenization schematic is proposed for the inverse estimation of the homogenized elastic properties of the effective cluster. Through the proposed multiscale homogenization schematic, the homogenized elastic properties of the effective cluster are determined, and fitted as the function of the radius of cluster at fixed volume fraction and radii of nanoparticles, where the cluster of nanoparticles is simplified as the spherical inclusion with homogeneous and isotropic elastic properties. By using the aforementioned effective interphase percolation model, the homogenized elastic properties of volume element that includes a single cluster of nanoparticles are obtained. Finally, it is verified that the effective cluster model is applicable to the polymeric nanocomposites including a number of clusters.

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Title: An Investigation into the Effect of Molybdenum on Interfacial Properties of TiC/Steel Composite through Atomistic Simulation

Author(s): *Seungchan Cho, Ilguk Jo, Sang-Kwan Lee, Sang-Bok Lee, *KIMS*; Jaekwang Lee, *Pusan National University*; Jae Hyun Park, *Gyeongsang National University*.

SKD11 (AISI D2) tool steel has been widely used for tools, metallic molds, rolls, and dies for machining processes because of its favorable mechanical properties, such as high toughness and hardness, as well as its overall wear resistance. The durability of tool steels has attracted great attention in recent years due to growing demands for processing high-strength materials. (MMCs) have become the focus of intensive research and development due to their high specific modulus and strength, thermal stability and weight reduction. Steel based alloys are by far the most widely used as metallic materials in MMCs because of their low cost and good mechanical properties. TiC is a well-known reinforcement in steel composites because of its desirable characteristics, such as its high melting point, low density, high elastic modulus, and good wettability with iron and steel matrices. In the present study, TiC–SKD11 composites, which are of great interest due to their wide range of industrial applications, were fabricated, and the effects of TiC–SKD11 interface on the mechanical properties of the composite were studied in detail. Mechanical properties of the composite were dramatically increased compared with SKD11. As a result of experimental and computational analysis based on density-functional theory of TiC/SKD11 interface, Molybdenum (Mo) enhances the interfacial bonding strenth of TiC particles to the matrix steel, due to its tendency to diffuse into the TiC particle surface for generating MoC phase.

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Title: Space–Time Least-Squares Petrov-Galerkin Projection in Nonlinear Model Reduction

Author(s): *Youngsoo Choi, Kevin Carlberg, *Sandia National Laboratories*.

Reduced-order models (ROMs) of nonlinear dynamical systems are essential for enabling high-fidelity computational models to be used in many-query and real-time applications such as uncertainty quantification and design optimization. Such ROMs reduce the dimensionality of the dynamical system by executing a projection process on the governing system of nonlinear ordinary differential equations (ODEs). The resulting ROM can then be numerically integrated in time. Unfortunately, many applications require resolving the model over long time intervals, leading to a large number of time instances at which the fully discretized model must be resolved. As such, the number of time instances required for the ROM simulation remains large, which can limit its realizable computational savings. Space–time ROMs have been devised for computational models that have been developed using a space–time finite-element formulation [2]. Unfortunately, many practical computational models are constructed using a spatial discretization (which yields a parameterized system of ODEs) followed by time integration with a linear multi-step method or Runge–Kutta scheme; such space–time ROMs cannot be applied for these models. To address this, we propose to apply a space–time projection to nonlinear ODE models, which are resolved in time using implicit time-integration schemes. The method adopts the least-squares Petrov–Galerkin (LSPG) formulation that underlies the Gauss–Newton with approximated tensors (GNAT) method [1]. The proposed technique executes the following steps: (1) introduce a low-dimensional (spatiotemporal) basis for the state (over all time), (2) apply implicit time integration to the system of nonlinear ODEs, (3) minimize the sum of squares of discrete residuals arising over all time steps. The technique also introduces hyper–reduction (via collocation or gappy POD) with an attendant spatiotemporal sample mesh in order to realize computational savings. [1] K. Carlberg, C. Farhat, J. Cortial, and D. Amsallem. The GNAT method for nonlinear model reduction: effective implementation and application to computational fluid dynamics and turbulent flows. Journal of Computational Physics, 242:623-647, 2013 [2] M. Yano. A space–time Petrov-Galerkin certified reduced basis method: application to the Boussinesq equations. SIAM Journal of Scientific Computing, 36.1:A232-A266, 2014

14th U.S. National Congress on Computational Mechanics
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Title: Removing Mesh Bias in a Cohesive Surface Element Approach for Two- and Three- Dimensional Mixed-Mode Fracture Analysis

Author(s): *Habeun Choi, Kyoungsoo Park, *Yonsei University*.

In the cohesive surface element approach, a crack propagation direction is generally limited to the boundary between continuum elements, which can cause inaccurate computational results. In order to overcome mesh bias issues and represent an accurate crack path in mixed-mode fracture simulation, an element splitting technique[1] is proposed in conjunction with an extrinsic cohesive zone model. The maximum principal stress criterion is used to determine the crack growth direction. For a given crack propagation direction, a continuum element is split and a cohesive element is adaptively inserted. A virtual mesh grid technique is introduced for an accurate stress field evaluation around a crack tip region. The topology-based data structure (TopS)[2] is utilized to update local element connectivities, and the generalized displacement control[3] is employed to capture softening behaviors. The proposed computational framework is verified and validated by illustrating mixed-mode fracture examples. In a two-dimensional case, a single edge notched tension test is simulated for a material with microstructure. Multiple crack initiation, crack branching and coalescence are represented using the proposed framework. In three-dimensional case, a mode I crack propagation problem is illustrated to verify the consistency of the element splitting scheme. Then, a four-point-shear test problem is investigated. Keywords: crack path representation, extrinsic cohesive zone model, mixed-mode fracture, microstructure References [1] H. Choi, K. Park, Removing mesh bias in mixed-mode cohesive fracture simulation using element split and stress recovery, Computer Methods in Applied Mechanics and Engineering, 2017, in preparation. [2] W. Celes, G. H. Paulino, & R. Espinha, A compact adjacency-based topological data structure for finite element mesh representation, International Journal for Numerical Methods in Engineering, 2005, 64 (11), pp. 1529-1556. [3] Y. B. Yang , L. J. Leu , & Judy P. Yang, Key Considerations in tracing the postbuckling response of structures with multi winding loops, Mechanics of Advanced Materials and Structures, 2007, 14(3), pp. 175–189.

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Title: Molecular Modeling of Cross-Linked Phthalonitrile (PN) Polymers: A Study of the Mechanical and Electromagnetic Properties of Cross-Linked PN

Author(s): Qingsong Tu, *UC Berkeley*; *Janel Chua, *National University of Singapore*.

Polymeric based electromagnetic interference (EMI) shielding materials have emerged as an attractive alternative to traditionally used metal based materials. In the past year, researchers have successfully demonstrated the synthesis of a novel Phthalonitrile (PN)-based carbon foam; a polymeric foam material that exhibited both high EMI shielding effectiveness and specific mechanical strength. In this work, Molecular dynamics and molecular mechanics are used to establish well equilibrated molecular models of the Phthalonitrile system with a range of crosslink densities using a consistent valence force field. Molecular dynamics simulations are subsequently used to study some important properties, including compressive strength and dielectric constant. Both carbonization and addition of fillers were also examined to study the change of dielectric constant. During the process of carbonization, we verified that the formation of sp2 carbon structures increases the conductivity of the material. The transition of the polymer between insulator and conductor during carbonization was found to be highly related to the sp2 carbon structures. Finally, we studied the manner in which the dielectric constant of the cross-linked polymer changes with addition of fillers, an alternative way of achieving high dielectric constant and high EMI shielding effectiveness without the potentially costly process of carbonization.

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Title: Atomic-Microscale Modeling of Phonons in the Molecular Crystal RDX

Author(s): Francis VanGessel, *Peter Chung, *University of Maryland*.

RDX is an energetic molecular crystal in which lattice vibrations are believed to play a large role in initiation mechanics. In addition to the short-ranged covalently-bonded interactions, which are found in the majority of solids in which phonons have been investigated in the literature, non-bonded long range forces play a significant role in the structural properties of RDX and other emerging materials such as so-called van der Waals solids. Here, we study of the microscale thermal transport properties of RDX via atomic and phonon Boltzmann transport equation modeling, using a recently developed anisotropic full Brillouin Zone model [1]. The full Brillouin zone model employs atomic models for its parameterization, allows for simulation of all lattice vibrational modes, and inherently captures anisotropy in thermal flow. Thus we will demonstrate how phonons are transported within the RDX crystal. In addition to addressing important questions regarding the behavior of phonons in RDX, this talk will further describe heat conduction mechanisms within anisotropic materials. Such mechanisms have become increasingly of interest due to the unique modalities of heat flow they enable, particularly flow-directional bias, and due to the promise of predictable and controllable thermoelectric behaviors at submicron scales. As such, new techniques have been developed to model these materials. However there still exist knowledge gaps regarding, for example, heat flow in non-covalently bonded crystals such as RDX where van der Waal's and Coulombic forces play a large role. Thus the aim of this talk is to both demonstrate anisotropic heat flow in RDX and by doing so improve model descriptions of phonon processes in non-covalently bonded crystals. [1] F. VanGessel and P. Chung, "An anisotropic full Brillouin zone model for the three dimensional phonon Boltzmann transport equation", Computer Methods in Applied Mechanics and Engineering, vol. 317, pp. 1012-1036, 2017.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Adaptive Multiscale Methods for Heterogeneous Flows

Author(s): *Eric Chung, *CUHK*.

The construction of local reduced-order models via multiscale basis functions has been an area of active research. In this talk, we present online multiscale basis functions which are constructed using the offline space and the current residual. Online multiscale basis functions are constructed adaptively in some selected regions based on our error indicators. We derive an error estimator which shows that one needs to have an offline space with certain properties to guarantee that additional online multiscale basis function will decrease the error. This error decrease is independent of physical parameters, such as the contrast and multiple scales in the problem. The offline spaces are constructed using Generalized Multiscale Finite Element Methods (GMsFEM). We show that if one chooses a sufficient number of offline basis functions, one can guarantee that additional online multiscale basis functions will reduce the error independent of contrast. We note that the construction of online basis functions is motivated by the fact that the offline space construction does not take into account distant effects. Using the residual information, we can incorporate the distant information provided the offline approximation satisfies certain properties. Our numerical results show that if the offline space is sufficiently large (in terms of the dimension) such that the coarse space contains all multiscale spectral basis functions that correspond to small eigenvalues, then the error reduction by adding online multiscale basis function is independent of the contrast. We discuss various ways computing online multiscale basis functions which include a use of small dimensional offline spaces. This work is partially supported by Hong Kong RGC General Research Fund (Project: 14317516).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Implementation of Discontinuous Skeletal Methods on Arbitrary-Dimensional, Polytopal Meshes Using Generic Programming

Author(s): *Matteo Cicuttin, Alexandre Ern, *CERMICS - École des Ponts*; Daniele Di pietro, *Institut Montpelliérain Alexander Grothendieck*.

Discontinuous Skeletal (DiSk) methods present several attractive features. The most important ones are that the mathematical construction is dimension-independent, that arbitrary polynomial orders can be used, and that general meshes, including polytopal cells and non-matching interfaces, are supported. Positioning unknowns at mesh faces is also a natural way to express locally in each mesh cell the fundamental balance properties satisfied by the boundary-value problem at hand. We refer to [1] for the devising and analysis of Discontinuous Skeletal methods. Implementations of DiSk methods, at least in principle, should conserve dimension-independency and cell-shape-independency: a single piece of code should be able to work in any space dimension and to deal with any cell shape. It is not common, however, to see this approach in software. In the vast majority of the cases, the codes are capable to run only on a few specific kinds of mesh, or only in 1D or 2D or 3D. On the one hand, this can happen because a fully general tool is not needed. On the other hand, the programming languages commonly used by the scientific computing community (in particular Fortran and Matlab) are not easily amenable to an implementation which is general and efficient at the same time. The usual approach, in conventional languages, is to have different versions of the code, but this results in non-trivial software maintenance issues. Generic programming offers a valuable tool to address the above issues: by writing the code generically, it is possible to avoid making assumptions neither on the dimension (1D, 2D, 3D) of the problem, nor on the kind of mesh. In some sense, writing generic code resembles writing pseudocode: the compiler will take care of giving the correct meaning to each basic operation. The resulting code, however, will remain efficient despite the generality since generic programming, being a static technique, allows to realize abstractions that do not penalize the performance at runtime. In this work, we show how DiSk methods can be implemented in a generic manner [2]. We implemented a generic library, DiSk++ [3], and we report benchmarking results on the Poisson problem, on different 2D and 3D meshes. [1] D. Di Pietro and A. Ern, A hybrid high-order locking-free method for linear elasticity on general meshes, Comp. Meth. Appl. Mech. Eng., 283, 1--21 (2015) [2] https://hal.archives-ouvertes.fr/hal-01429292 [2] https://github.com/datafl4sh/diskpp

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Title: A Stochastic Approach for Modeling Dynamic Fracture of Quasi-Brittle Materials

Author(s): *Philip Clarke, *University of Tennessee Space* ; Reza Abedi, *University of Tennessee Space Institute*; Robert Haber, *University of Illinois at Urbana-Champaign*; Katherine A. Acton, Sarah C. Baxter, *University of Saint Thomas*.

Hydraulic fracturing has been the most common approach to stimulate tight formations. The geometry of the wellbore and the time history of the hydraulic loading play important roles in induced fracture patterns. For example, generating multiple perforations in a wellbore to enhance its hydrocarbon recovery is nowadays attracting more attention. The increased number of fractures can potentially enhance the yield of a reservoir by increasing the regions affected by hydraulic fractures. However, in practice many of the initial perforations do not result in any substantial hydraulic crack propagation. Dynamic stimulation methods are often associated with explosive or propellant methods. These approaches are typically performed without any initial perforations. However, recent studies show that by using a hybrid approach, in which similar to hydraulic fracturing there are some initial perforations but for these high loading rate conditions, all perforations can be activated, thus affecting larger areas of the reservoir. We study the conditions for which the initial perforations become effective and propagate in rock. We combine the asynchronous spacetime discontinuous Galerkin method with an interfacial damage model in our fracture simulations. Mesh adaptive schemes are used to align crack trajectories with inter-element boundaries. We consider loading rates ranging from 10 microseconds to 1 second. The first few high loading rates are hypothetical and are included to better demonstrate the effect of fracture strength randomness on fracture response. The loading rates from 1 to 100 milliseconds correspond to the aforementioned hybrid methods, while lower rates can be associated with very early stages of hydraulic fracturing. Our numerical results show that at low loading rates only a few of the initial perforations become active. As the loading rate increases, more perforations become active until ultimately all result in crack propagation. Moreover, higher loading rates affect larger zones for each of the initial perforations by dynamic fracture features such as microcracking and crack bifurcation. In-situ stress anisotropy has an adverse effect in that it prohibits activation of more perforations even at higher loading rates. Finally, we study the effect of spatial inhomogeneity of fracture strength on generated fracture patterns; as the loading rate increases a deterministic model, which assumes fracture strength is spatially uniform, starts to induce more microcracking and crack branching events. Accordingly, these studies imply the high impact of local material inhomogeneities on fracture response, particularly at high loading rates.

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Title: A Stabilised Cut Finite Element LaTin Method for Multiple Unilateral Contact Problems

Author(s): *Susanne Claus, *Cardiff University*; Pierre Kerfriden, *Cardiff University* .

In this presentation, we introduce a cut finite element method for unilateral contact problems. More specifically, we will present a stabilised scheme to simulate contact problems between two or more linear elastic bodies. In this context, the finite element space needs to be enriched to allow for jumps in the displacement over the unfitted interfaces. The CutFEM approach [1] does this by doubling elements that are cut, and enforcing kinematic conformity though a Nitsche formulation. In our contribution, we follow a different route that relies on the LaTIn method [3]. This mixed formulation discretises both interface fields and fluxes as unknowns, and searches for them iteratively. We stabilise our scheme using ghost penalty regularisation [2]. In the presentation, we will introduce our proposed combination of CutFEM and the LaTIn algorithm to solve unilateral contact problems. We will pay close attention to the discretisation of the interface fields. We will prove numerically that our formulation converges optimally with mesh refinement, and that the condition number remains well-behaved. We will also present the capabilities of our numerical implementation of this new strategy, which can deal with complex 3D problems, including contact between multiple bodies at a single point (i.e. multiple junction) such as braided composites. [1] Burman, E. and Claus, S. and Hansbo, P. and Larson, M. G. and Massing, A. CutFEM: discretizing geometry and partial differential equations. Int. J. Numer. Meth. Engng. 104:472--501 (2015). [2] Burman, E. Ghost penalty. C. R. Math. Acad. Sci. Paris. 348:1217--1220 (2010). [3] Ladevèze, P. Nonlinear Computational Structural Mechanics - New Approaches and Non-Incremental Methods of Calculation. Springer Verlag, (1999).

14th U.S. National Congress on Computational Mechanics
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Title: Prototyping the Next Generation of Aria

Author(s): *Jonathan Clausen, Chris Forster, David Noble, Christian Trott, Si Hammond, Mark Hoemenn, Paul Lin, *Sandia National Laboratories*.

The SIERRA Aria thermal/fluid application is a very large, complex production code base developed over the past few decades and contains a variety of C++ styles up to C++11. Subsequently, many object-oriented mechanisms and virtual calls are utilized throughout the code to perform core computational kernels. Porting Aria to next-generation platforms, including GPUs, will require a significant effort. To enable rapid prototyping of new code designs that make use of as much existing framework as possible, Ariamini was created using a core subset of the Aria application. We are able to explore strategies to provide portable performance on newer architectures while maintaining a clean, sustainable code base prior to implementing the modifications in the Aria production code. In this talk we will present work on the use of Kokkos data structures and parallel constructs, SIMD data types, as well as other code structures within Ariamini in order to demonstrate the impact on performance when running on CPU architectures such as Intel Sandy Bridge, Haswell and Knights Landing processors, as well as GPU-based architectures. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
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Title: Numerical Modeling of Inertial Focusing Effects in Curved Microfluidic Flows

Author(s): *Liviu Clime, Xuyen Dai Hoa, Keith J. Morton, *National Research Council (CA)*.

Among the variety of useful effects relying on fluid inertia at the microscale, inertial focusing has become lately an invaluable tool for filtration and size-based particle separation [1]. Driven by lateral migration of buoyancy neutral particles across undisturbed fluid streamlines and manifested by focusing at well-defined outlet positions, the effect is exploited in many applications ranging from membrane-less environmental cleanup and physiological fluid processing to high-throughput bioparticle separation and sheathless flow cytometry. Recent advances in numerical modeling based on techniques such as asymptotic expansions, lattice-Bolzmann and finite element analysis have contributed to a more thorough understanding of the underlying physics of this phenomenon and gave useful insights into the dynamics of individual particles. However, practical applications require deeper understanding of large assemblies of particles as well as design rules to relate particle distributions to the geometry and physical parameters of the microfluidic flows. While single-particle problems can be addressed by implementing liquid-solid interaction algorithms directly into CFD solvers, the many-particle problem is more challenging especially when a large number of particles is envisaged. In this presentation we describe our contribution towards the kinematics of large assemblies of buoyancy neutral particles suspended in inertial flows at relatively low Reynolds numbers. The approach consists mainly of decoupling the liquid flow from the dynamics of suspended non-interacting particles [2] by neglecting the influence of the particle motion on the liquid flow. The resulting hybrid model is able to predict accurately particle trajectories in both straight and curving microfluidic flows as confirmed by fluorescence and confocal microscopy measurements [2]. We also highlight the accuracy of the proposed mathematical algorithm by reproducing three particle focusing regimes that may occur in the twin tubular pinch effect [2]: (i) subcritical, where inertial migration is relatively weak, (ii) critical where lateral migration forces are the same order of magnitude as Dean-induced drag, and (iii) supercritical where Dean-induced drag is completely exceeded by lateral migration effects. Moreover, explicit particle distributions and insights into the spatial topology and time evolution of statistically relevant particle clouds involved in a lateral migration process are presented along with related experimental measurements. We conclude the presentation by discussing possible extensions of the model to microfluidic flows in channels of arbitrary shape with special emphasis on rectangular cross-section microchannels. Design rules, overall efficiency and limitations in size separation applications will be discussed and practical examples will be given. REFERENCES: [1] D. Di Carlo, Lab Chip 2009, vol. 9, p. 3038 [2] L. Clime, K. J. Morton, X. D. Hoa, and T. Veres, Nature Sci. Rep. 2015, vol. 5, p. 9765

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Title: Multiscale Methods for Uncertainty Propagation for Polycrystalline Aluminum 6061-T6

Author(s): *Peter Coffin, John Emery, Brian Robbins, Jay Carroll, *Sandia National Labs*.

We strive to develop an approach to predict multiscale reliability in applications where ductile crack nucleation is the predominant mechanism of interest. Existing numerical methods and constitutive models are coupled in a framework that allows for efficient uncertainty propagation and therefore the study of reliability. A number of simplifications must be utilized to obtain a computationally tractable approach. Stochastic reduced-order models are used to aid in simplifying the uncertainty propagation. In this talk we present the multiscale modeling approach and methods used to study microstructure behavior in the context of uncertainty analysis. For this work a polycrystal model of microstructure is generated based on average grain morphology, including a second phase, and with a stochastic random field model to represent texture. This microstructure model is then coupled to an engineering scale simulation of a multiply-notched tensile specimen. We will discuss the impacts of meshing considerations (for polycrystal generation) and multiscale coupling on the resulting reliability calculations.

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Title: Variational Multiscale Error Estimators for the Uncertainty Quantification of Mesh Discretization Errors

Author(s): *Oriol Colomés, Guglielmo Scovazzi, *Duke University*.

When trying to quantify the uncertainty of a given simulation, one has to identify the sources of such uncertainty. These sources can be classified into input uncertainty, numerical approximation uncertainty, or modelling uncertainty. In this work we focus on the numerical approximation uncertainty, but it is well known that the accuracy of the numerical approximation methods depends on the input parameters. For example, we could have uncertainty on the properties of the material being simulated. In this work we firstly assess the behaviour of some existing Variational Multiscale (VMS) error estimators for the Uncertainty Quantification (UQ) of Mesh Discretization Error (MDE) under uncertain input parameters. The VMS error estimators are typically described in a Finite Element (FE) framework and, since they involve second order spatial derivatives, they are hardly extensible to Finite Volume (FV) methods. In order to overcome this difficulty, we also propose new VMS error estimators that can be easily used in a FE or FV context. The VMS error estimators are analysed for canonical convection-diffusion-reaction problems and then extended to turbulent incompressible flow problem.

14th U.S. National Congress on Computational Mechanics
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Title: Addressing Customer Needs Through Open Processes and Software

Author(s): William Schroeder, *Kitware, Inc*; *Thomas Corona, *Kiltware, Inc.*.

The larger part of the software market is services, in particular customized workflows to meet research and enterprise needs. Effective engagement requires open platforms that can be readily combined into customized solutions. Such platforms also leverage the strength of broader, worldwide communities to deliver cutting edge innovation. In this presentation we discuss approaches to developing open platforms and software tools, and provide case studies that describe successes and failures.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A New Godunov-Type Scheme for the Two-Dimensional Lagrangian Hydrodynamics

Author(s): *Théo Corot, *CNAM*; Bertrand Mercier, *CNAM and CEA/INSTN*.

Steam explosion is a fast vaporization of water, which leads to pressure shocks. This phenomenon is of interest in the nuclear safety domain. Indeed, during a core-meltdown crisis, molten fuel rods interacting with water could lead to steam explosion. Consequently we want to evaluate the risks created by this phenomenon. In order to simulate this problem, one need a multi-fluid model, which will be the Euler equations, and a numerical scheme. These equations will be used in the Lagrangian framework which is convenient to compute multi-material flow. Indeed Lagrangian methods have the advantage of naturally capturing interfaces between materials. Our target is to develop a scheme for two-dimensional Lagrangian hydrodynamics. We choose to use a Godunov type scheme which have the quality of capturing shocks without needing artificial viscosity. However, such methods also require the definition of node velocities to move the mesh. Consequently we use nodal fluxes. Therefore a nodal solver, which permits to compute node velocities and pressures knowing physical variables in surrounding cells, is needed. The development of such schemes has been initiated by Mazeran and Després [1] and pursued by Maire [2] who noticed a strong sensitivity of the first scheme to cell aspect. However, the nodal solvers they use can give an incorrect direction of node velocities in the simple case of a one-dimensional Riemann problem. Consequently we develop a new nodal solver, which uses Després-Mazeran's ideas with a continuous point of view around the node. Our nodal solver is a two-dimensional generalization of the one-dimensional acoustic solver. Our approach leads to a nodal solver, which only depends on the angular repartition of physical variables around the node and not on characteristic lengths of the mesh. Consequently, it always recover the right direction of the velocity when one consider one-dimensional Riemann problem. Furthermore, our scheme is conservative since we define a unique pressure at each node. Moreover, numerical results show our scheme reduces symmetry errors and has low dissipation. We also prove that it satisfies a weak-consistency property. Finally we focus our interest on applying this scheme to simulation of steam explosion. [1] Després, B., Mazeran, C.: Lagrangian gas dynamics in two dimensions and lagrangian systems. Archive for Rational Mechanics and Analysis. 2005. [2] Maire, P.H.: A high-order cell-centered lagrangian scheme for two-dimensional compressible fluid flows on unstructured meshes. Journal of Computational Physics. 2009.

14th U.S. National Congress on Computational Mechanics
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Title: The Impact of Automated, Unstructured Meshing on the Use of CFD in Industry

Author(s): *David Corson, *Altair Engineering*.

The use of Computational Fluid Dynamics within industry has increased dramatically over the past 20 years. A number of key technologies have contributed to this growth. Advancements in compute power have played a major role in enabling small to mid-sized companies to leverage CFD, and at the same time, the advancements in unstructured meshing technology have significantly reduced the learning curve for engineers to adopt CFD and become proficient users. Professor Shepard's contributions to the state of the art in meshing technology for the basis for much of the meshing technology in place in industry today. This technology, when coupled with solver technology that efficiently leverages unstructured meshes, has given rise to the successful deployment of CFD in many businesses. It has enabled novice users to quickly learn to use CFD, expert users to fully automate their analyses, and impacted the industry greatly. In this talk, an overview on the use of CFD in industry will be provided, followed by a discussion on how unstructured meshing has changed the workflows of CFD users. The talk will conclude with some examples of industries that are successfully leveraging CFD using unstructured meshing.

14th U.S. National Congress on Computational Mechanics
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Title: An Arbitrary Lagrangian-Eulerian Approach to Acoustic Streaming

Author(s): *Francesco Costanzo, Nitesh Nama, *Penn State University*; Tony Huang, *Duke University*.

Over the past few decades, microfluidics has received significant interest owing to its numerous applications in biology, chemistry, and medicine. In these fields, microfluidic devices and techniques offer significant advantages over the traditional ones in terms of miniaturization, low-cost, automation, precise microenvironment control, and reduced sample consumption. However, there are significant challenges to overcome in the use of microfluidic devices in key applications that require pumping and mixing. To overcome these challenges, as well as to achieve novel functionalities, researchers have integrated different physics into the microfluidic platforms such as electrokinetics, chemistry, optics, biotechnology, etc. Among these, microacoustofluidics, which refers to the merger of acoustics and microfluidics, has shown great promise. These systems are typically characterized by the propagation of high-frequency acoustic waves through fluids. The wave propagation not only induces a corresponding high-frequency response of the fluid, but also a slow mean flow through a nonlinear phenomenon referred to as acoustic streaming. We adopt an ALE perspective in the characterization of acoustic streaming flows. In our formulation we build an explicit separation of time-scales resulting in two subproblems: a first-order problem, formulated in terms of the fluid displacement at the fast scale, and a second-order problem formulated in terms of the Lagrangian flow velocity at the slow time scale. We then proceed to a rigorous time-averaging procedure, which, contrary to more familiar Eulerian formulations, yields an intrinsically steady second-order problem with exact boundary conditions at the oscillating walls. The second-order problem is solved directly for the Lagrangian velocity so that the proposed formulation does not need to employ the notion of Stokes drift, or any associated post-processing to identify the mean particle velocity field. This greatly facilitates a direct comparison with experiments. Because the first-order problem is formulated in terms of the displacement field, our formulation is directly applicable to more complex fluid-structure interaction problems in microacosutofluidic devices. In addition to the formulation, we present numerical results for test cases where the Eulerian flow velocities exhibit several non-physical features that are not observed in the corresponding Lagrangian flow velocities, indicating that a formulation based on the Lagrangian flow velocity is much more favorable and readily interpretable.

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Title: High-Fidelity Simulation of a Golf Ball Trajectory Using a High-Order Overset Method

Author(s): *Jacob Crabill, Freddie Witherden, Antony Jameson, *Stanford University*.

Grid generation is commonly a bottleneck in the use of high-order finite-element methods on complex geometry. Not only is a properly curved boundary representation required to avoid serious degradation in accuracy, high-order methods also tend to be more sensitive to the highly-skewed elements that often appear near corners or in grids around multiple boundaries. Additional complications are introduced when moving boundaries are desired. The overset grid approach provides an efficient means of tackling the problems of both grid generation and grid motion. By generating a separate grid around each body of interest in combination with a structured background grid, grid quality around complex geometries can be improved while taking less effort to generate. Further, moving grids are handled quite naturally within the overset framework. In this presentation, we will address our work on efficient high-order overset CFD by applying it to the problem of modeling the full trajectory of a spinning golf ball. The overset golf ball grid is created by combining a structured multi-block grid generator with a mesh agglomeration utility to create high-order curved hexahedrons. The simulation is performed using our GPU-accelerated Flux Reconstruction solver, which has been extended to handle overset grids through the use of an external domain connectivity library. Our previous work on applying the overset approach to high-order methods showed that the accuracy of a simulation is not significantly impacted over the use of a single grid [1]. Now, by developing novel algorithms to perform the overset connectivity and interpolation in parallel on the GPU we have obtained a substantial speedup over typical serial CPU-based algorithms, thus enabling the efficient simulation of large cases. We will show that this high-order overset method allows for the accurate simulation of moving objects, without a significant performance penalty over static grids. [1] Crabill, J., Jameson, A. and Sitaraman, J.: A High-Order Overset Method on Moving and Deforming Grids. AIAA 2016-3225, AIAA Aviation, AIAA Modeling and Simulation Technologies Conference, 13-17 June 2016, Washington, DC.

14th U.S. National Congress on Computational Mechanics
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Title: Capturing the Collaborative Strengthening Effects of Work Hardening and Precipitation Hardening with Dislocation Dynamics

Author(s): *Joshua Crone, Jaroslaw Knap, *US Army Research Laboratory*.

The strength of crystalline material is controlled, to a large extent, by the motion of dislocations. In materials with a high density of microstructural features, the motion of dislocations is restricted, resulting in increased strength. The small scale plasticity occurring in the vicinity of microstructure is a fundamentally multiscale phenomena. Bridging the characterization of individual dislocations at the atomistic scale with the macroscopic plastic response from cooperative dislocation motion at the continuum scale remains an open challenge. A method well suited for bridging this gap is discrete dislocation dynamics (DDD), where plasticity is explicitly captured by the motion of individual dislocations. In this work, we present a scalable algorithm for modeling DDD with microstructural effects. The method involves coupling a highly parallel DDD simulator for bulk materials (ParaDiS) with a highly parallel finite element method (FEM) solver to capture microstructual effects. We first use the coupled DDD-FEM simulator to model the strengthening effects of a periodic array of nanoscale voids, elastically homogeneous precipitates, and elastically inhomogeneous precipitates. To explore the collaborative effects of dislocation and obstacle hardening mechanisms in realistic geometries, we perform multiple simulations with random configurations of dislocations and precipitates. By averaging over multiple runs with smaller system sizes, we find the mean strengthening effect to be in excellent agreement with larger system size simulations requiring considerable more computational resources.

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Title: Multiscale Diffusion Method for Simulations of Long-Time Defect Evolution

Author(s): *William a. Curtin, *EPFL STI IGM LAMMM*.

In many problems of interest to materials scientists and engineers, the evolution of crystalline extended defects (dislocations, cracks, grain boundaries, interfaces, voids, precipitates) is controlled by the flow of point defects (interstitial/substitutional atoms and/or vacancies) through the crystal into the extended defect. Precise modeling of this behavior requires fully atomistic methods in and around the extended defect, but the flow of point defects entering the defect region can be treated by coarse-grained methods. Here, a multiscale algorithm is presented for achieving this coupling. Specifically, direct accelerated molecular dynamics (AMD) of extended defect evolution is coupled to a diffusing point defect concentration field that captures the long spatial and temporal scales of point defect motion in the presence of the internal stress fields generated by the evolving defect. The algorithm is applied to study vacancy absorption into an edge dislocation in aluminum where vacancy accumulation in the core leads to nucleation of a double-jog that then operates as a sink for additional vacancies; this corresponds to the initial stages of dislocation climb modeled with explicit atomistic resolution. The method is general and so can be applied to many other problems associated with nucleation, growth, and reaction due to accumulation of point defects in crystalline materials.

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Title: Surface Sensing of Atomic Behavior of Polymer Nanofilms via Molecular Dynamics Simulation

Author(s): *Ling Dai, *Institute of High Performance Computing, Singapore*.

Surface-sensing devices such as atomic force microscope have been widely used to characterize the surface structure and properties of nanoscale polymer films. However, using molecular dynamics simulations, we show that there is intrinsic and unavoidable inelastic alteration at polymer surfaces induced by the sensing tip. For linear chain polymers like perfluoropolyether, such tip-induced alternation arises from the differences in van der Waals interactions between different atomic species in the polymer and in the sensing tip, leading to atomic shuffling. Such shuffling re-organizes the surface morphology into a layered profile, which causes inelastic alternation to molecular structures. Furthermore, the mechanical properties at and near the polymer surface is also softened, allowing a more endurable response to the outer enforcements. Meanwhile, for those aromatic chain polymers like epoxy, the intrinsic deformation is depicted as the intra-chain rotation of aromatic rings and kinking of linear atomic connections, which also downgrades the surface stiffness. With larger contact area, the interfacial adhesion and friction are expected to be enhanced. The present work highlights the need to reinterpret the data obtained from surface-sensing tests by considering this intrinsic inelastic deformation occurring at and near polymer surfaces.

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Title: Phase-Field Free Energy and Boundary Force for Molecular Solvation

Author(s): *Shibin Dai, *New Mexico State University*; Bo Li, *University of California San Diego*; Jianfeng Lu, *Duke University*.

We discuss a phase-filed variational model for the solvation of charged molecules with implicit solvent. The solvation free-energy functional of all phase fields consists of the surface energy, solute excluded volume and solute-solvent van der Waals dispersion energy, and electrostatic free energy. The last part is defined through the electrostatic potential governed by the Poisson-Boltzmann equation in which the dielectric coefficient is defined through a phase field. We prove Gamma- convergence of the phase field free-energy functional to its sharp-interface limit. We also define the dielectric boundary force for any phase field as the negative first variation of the free-energy functional, and prove the convergence of such force to the corresponding sharp-interface limit.

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Title: An Adaptive hp-Refinement Strategy with Computable Guaranteed Error Reduction Factors

Author(s): *Patrik Daniel, Iain Smears, Martin Vohralík, *Inria Paris*; Alexandre Ern, *Université Paris-Est, CERMICS (ENPC)*.

We propose a new practical adaptive refinement strategy for hp-finite element approximations of elliptic problems. Following some recent theoretical developments in polynomial-degree-robust a posteriori error analysis, we solve two complementary classes of discrete local problems on the vertex-based patches. The first class involves the solution on each patch of a mixed finite element problem with homogeneous Neumann boundary conditions, which leads to an H(div,Ω)-conforming equilibrated flux. This in turns yields a guaranteed upper bound on the error and serves to mark elements for refinement via a Dörfler bulk criterion. The second class of local problems involves the solution, on each marked patch only, of two separate primal finite element problems with homogeneous Dirichlet boundary conditions, which serve to decide between h-, p-, or hp-refinement. Altogether, we show that these ingredients lead to a computable error reduction factor; we guarantee that while performing the hp-adaptive refinement as suggested, the error will be reduced at least by this factor on the next hp-mesh. In a series of numerical experiments in two space dimensions, we first study the accuracy of our predicted reduction factor: in particular, we measure the ratio of the predicted reduction factor relative to the true error reduction, and we find that it is very close to the optimal value of one for both smooth and singular exact solutions. Finally, we study the overall performance of the proposed hp-refinement strategy on some test cases, for which we observe effectivity indices very close to one and exponential convergence rates.

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Title: Pyramid and Degenerate Elements for Lumped Mass Explicit Methods in Nonlinear Solid Dynamics

Author(s): *Kent Danielson Danielson, Mark Adley, *US Army ERDC*.

Pyramid finite elements have become increasingly popular to facilitate meshing, due to their distinctive shape and innate ability to transition naturally between quadrilateral and triangular elemental faces. This is especially important for explicit time integration typically used for impact and blast analyses, as the alternative of constraints can be problematic for wave propagation behavior inherent to such applications. Although formulations to alleviate singularity problems near the apex node have existed for decades, pyramid elements are not available in typical explicit solid dynamics software. Several 5-node pyramid approaches are evaluated herein for suitability as transition elements in lumped mass explicit methods for nonlinear solid dynamics problems. Bedrosian rabbit function type elements are extended to explicit temporal methods by the development of mass lumping and critical time increment estimation schemes. Standard and uniform strain hexahedrons are also degenerated into a pyramid by nodal duplication in the connectivity, which is a modeling trick performed without coding changes. A focus of the study is on the viability of using only existing hexahedron capabilities typically available in many explicit codes. Performance is assessed in standard benchmark problems and practical applications using various elastic and elastic-plastic material models and involving large strains/deformations, severe distortion, and contact-impact. Examples first evaluate the elements on their own and then for the principal case as transitions within a hexahedral-dominant model. Row-summation mass lumping is shown to be the best method for any pyramid element approach, but it may require slight coding changes for degenerated hexahedrons. The results indicate that it may also be a good systematic method for mass lumping of general degenerate hexahedral types. The single quadrature point Bedrosian element is also found to be robust and the best performer, particularly requiring significantly fewer computations than the degenerated uniform strain hexahedron. If used properly, however, all element types are demonstrated to perform satisfactorily (and identically) and thus demonstrate their viability and benefits for practical applications using hexahedral-dominant meshing.

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Title: Simulation of Harmonic Shear Waves in the Human Brain and Comparison with Measurements from Magnetic Resonance Elastography

Author(s): *Nitin Daphalapurkar, Yang Li, K.T. Ramesh, *Johns Hopkins University*; Ruth Okamoto, Andrew Badachhape, Philip Bayly, *Washington University in St. Louis*.

Magnetic resonance elastography (MRE) provides a non-invasive method to characterize the mechanical response of the living brain subjected to dynamic loading conditions. In MRE, harmonic loading is applied to the human head and steady-state oscillations in the brain can be observed using a specialized pulse sequence in the magnetic resonance imaging (MRI) scanner. The peak magnitude of the strain is small and the excitation results in harmless deformation waves propagating through the brain. We hypothesize that the stiff membranes in the brain, falx and tentorium, modulate the resulting deformation field, hence, these membranes are essential anatomical sub-structures to include in computational models of brain injury. In this paper, we develop a computational model for the brain, with relevant substructures of the head based on MRI. Harmonic wave motions in a live human brain obtained in an MRE experiment were used to assess the accuracy of the computational model by comparing the measured and the predicted dynamic mechanical response of the brain. Quantitative comparison of strain field in simulations with measured data from MRE shows that the dynamic deformation of the brain tissue is responsive to changes in the viscoelastic properties of the brain. In addition, the results demonstrate the presence of falx membrane alters the spatial deformation field and peak strain amplitudes in the computational model of the brain.

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Title: Cohesive Fracture of Multilayered Beams Through a Homogenized Structural Theory

Author(s): *Hossein Darban, Roberta Massabò, *University of Genoa*.

Laminated and sandwich beams are being used frequently as structural components for applications in aggressive environments and under severe mechanical loadings. Due to the high interfacial tractions, multilayered systems are prone to delaminate. Delamination fracture in composite laminates may be studied through numerical tools by discretizing the domain in the in-plane and thickness directions and using cohesive-interface elements. The computational cost of this method depends on the discretization and may be very high for systems with many layers. This work proposes a novel homogenized approach for studying cohesive delamination fracture which avoids the through thickness discretization. The approach uses the multiscale structural model formulated in [1] for beams and plates with damaged interfaces which is based on the original theory in [2] for fully bonded plates. The model assumes a two-length scales zigzag displacement field described by global variables (first-order shear deformation theory) and local perturbations to account for discontinuities of the properties and interfacial displacement jumps. A homogenization technique is used to define the local variables as functions of the global variables so that the number of unknowns becomes independent of the number of layers and equal to that of the global model. Homogenized equilibrium equations and boundary conditions are obtained in terms of the global variables only, using the Principle of Virtual Work. In this work, the capabilities of the homogenized model to efficiently study mode II delamination cohesive fracture in delamination specimens are investigated. Different cohesive-traction laws are considered to examine different nonlinear fracture mechanisms. For bilinear cohesive laws, the structure is discretized only through the length, into regions separated by the cross sections at the traction-free and cohesive zone tips. These sections are initially unknown and are determined through an iterative solution process. The homogenized governing equations for the different regions are solved in closed-form and continuity and boundary conditions are imposed to obtain the solution. The fracture parameters are calculated and compared with solutions in the literature to assess the accuracy and reveal advantages and limitations of the approach. Acknowledgment Support by the U.S. Office of Naval Research no. N00014-14-1-0254 is acknowledged. References [1] Massabò R., Campi F. An efficient approach for multilayered beams and wide plates with imperfect interfaces and delaminations, Compos. Struct. 2014;116:311-324. [2] Di Sciuva M. Bending, vibration and buckling of simply supported thick multilayered orthotropic plates: an evaluation of a new displacement model, J. Sound Vibration 1986;105:425–442.

14th U.S. National Congress on Computational Mechanics
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Title: Preconditioners for the Boundary Element Method based on Hierarchical Matrices

Author(s): *Eric Darve, Pieter Coulier, *Stanford*; Toru Takahashi, *Nagoya University*.

The inverse FMM algorithm is an approximate linear solver which uses techniques from the fast multipole method to solve dense linear equations in O(N) flops (under certain low-rank assumptions). This is a multilevel algorithm, with a tunable accuracy epsilon used to approximate blocks in the matrix using low-rank factorizations. We will describe the algorithm and discuss its application to solving the Helmholtz equation using integral equations. We will discuss the performance of the algorithm as we vary the frequency, the boundary conditions, and geometry of the problem. The dependence of the rank used in the solver on the size of the object will be discussed.

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Title: Large Scale Electronic Structure Studies on the Energetics of Dislocations in Al-Mg Materials System and Its Connection to Mesoscale Models

Author(s): *Sambit Das, Vikram Gavini, *University of Michigan*.

We study the dislocation core in Aluminum and Magnesium using a local real-space formulation of orbital-free density functional theory, implemented using finite-element discretization. The framework affords the use of Dirichlet bulk boundary conditions enabling direct calculation of isolated dislocation core energetics. So far our studies on edge [1,2] and screw [3] dislocations in Aluminum, suggest that the core size—region with significant contribution of electronic effects to dislocation energetics—is around seven to ten times the magnitude of the Burgers vector. This is in stark contrast to estimates based on atomistic calculations. Interestingly, our study further indicates that the core-energy of both edge and screw dislocations are strongly dependent on external macroscopic strains. Similar studies in Magnesium are ongoing. Next, we use the electronic structure core energetics information to develop a continuum energetics model for a discrete dislocation network, which accounts for the core energy dependence on macroscopic deformations, and from the variations of the core energy with respect to the nodal positions of the network, we obtain the nodal core force [3] which can directly be incorporated into discrete dislocation dynamics frameworks. We analyze and classify the nodal core force into three different contributions based on their decay behavior. Two of these contributions, both arising from the core energy dependence on macroscopic deformations, are not accounted for in currently used discrete dislocation dynamics models which assume the core energy to be a constant excepting for its dependence on the dislocation line orientation. Using case studies involving simple dislocation structures, we demonstrate that the contribution to the core force from the core energy dependence on macroscopic deformations can be significant in comparison to the elastic Peach-Koehler force even up to distances of 10-15 nm between dislocation structures. Thus, these core effects, whose origins are in the electronic structure of the dislocation core, can play an important role in influencing dislocation-dislocation interactions to much larger distances than considered heretofore. [1] Iyer, M., Radhakrishnan, B., Gavini, V., 2015. Electronic-structure study of an edge dislocation in Aluminum and the role of macroscopic deformations on its energetics. J. Mech. Phys. Solids 76, 260-275. [2] Das, S., Iyer, M., Radhakrishnan, B., Gavini, V., 2016. Corrigendum to [1]. J. Mech. Phys. Solids 95, 428-429. [3] Das, S., and Gavini, V., Electronic-structure study of a screw dislocation in Aluminum and the role of macroscopic deformations on its energetics, (Under review at J. Mech. Phys. Solids).

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Title: Simulation of Steady-State Creep Behavior of Poly-Crystalline Solder Joints Based on an Anisotropic Multi-Scale Approach

Author(s): Qian Jiang, *Abhijit Dasgupta, *University of Maryland*.

Many solder alloys usually experience high homologous temperatures during typical application, because of their relatively low solidus temperatures. Thus, the time-dependent deformation, or creep is a common occurrence, even under modest stresses. Microelectronic interconnects made with Tin-rich solder alloys (e.g. SnAgCu) usually consist of just a few highly-anisotropic grains, making each joint unique and non-homogeneous. Thus simulation of solder deformation requires simulation of the full crystal structure. Anisotropic behavior of single Sn grain is modeled by a multi-scale method. Creep behavior of each grain is modeled with the load sharing between the pro-eutectic Sn phase and the surrounding eutectic Sn-Ag phase, within each grain. The eutectic phase, in turn, is modeled as a dispersion strengthened alloy, consisting of Sn matrix and nanoscale Ag3Sn IMC particles. The creep behavior of this dispersion-strengthened material is modeled with dislocation obstruction and recovery models. Model constants are calibrated by the secondary creep tests of single crystal SAC joints. For polycrystalline structure, there could be additional contribution from grain boundary sliding. Based on EBSD images of tested multi-crystal SAC joints, Finite Element models are created with the same crystal structure. Grain boundary sliding is incorporated with parametric model constants. Secondary creep behavior of poly-crystalline joints are analyzed under specific test conditions. The simulation outcomes are compared with the test results for each specimen, to infer the model constants for grain-boundary sliding.

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Title: MIT Uncertainty Quantification (MUQ): Flexible Software for Connecting Uncertainty Quantification Algorithms and Applications

Author(s): *Andrew Davis, Youssef Marzouk, *MIT*; Matt Parno, *CRREL*.

MIT Uncertainty Quantification (MUQ) is an open-source software package that provides tools for easily combining models with structure-exploiting uncertainty quantification (UQ) algorithms. Many UQ approaches are nonintrusive and can be applied to “black box” models. Implementing state-of-the-art UQ algorithms, however, can require advanced mathematical and/or software engineering knowledge; this complexity often prohibits users from applying UQ methods to their research. MUQ provides a framework for modelers-i.e., experts in their field who are not necessarily well versed in the complexities of developing UQ algorithms-to integrate their models with state-of-the-art UQ tools. Our framework also allows developers to combine many simple components into complex algorithms. For example, Markov chain Monte Carlo (MCMC) is divided into three subcomponents: (i) the chain, (ii) the kernel, and (iii) the proposal. Changing a subcomponent, e.g., introducing parallel MCMC chains, does not affect other subcomponents; the new parallel chain can use any proposal (e.g., adaptive Metropolis, MALA). Going further, one can introduce approximations of an expensive model into the MCMC transition kernel, and allow these approximations to be shared seamlessly across parallel chains. We have developed tools for MCMC sampling, constructing sparse polynomial chaos expansions, modeling random fields, performing inference and model learning with transport maps, optimization, and regression.

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Title: Advanced Finite Element Techniques Applied to Kohn-Sham Density-Functional-Theory: h-adaptive Matrix-Free Finite Element Energy Minimization and h-adaptive Partition-of-Unity Approach

Author(s): *Denis Davydov, *University of Erlangen–Nurembe*; Paul Steinmann, *University of Erlangen–Nuremberg*.

In this contribution we present our recent result for two different real-space finite-element based solution techniques of density functional theory. The first is the h-adaptive parition-of-unity approach [1,2] which enriches the finite element space with a-priori knowledge about the solution. The partition-of-unity method is equipped with an a posteriori error estimator, thus enabling implementation of error-controlled adaptive mesh refinement strategies. To that end, local interpolation error estimates are derived for the partition-of-unity method enriched with a class of exponential functions. The second is a matrix-free implementation of the steepest descent minimization of energy using finite elements preconditioned with geometric multigrids. Implementation details including various parallelization models (MPI, multithreading, SIMD) using the deal.II [3] library are presented. Advantages and disadvantages of the two methods are discussed. To exemplify the validity of the proposed approaches, accurate computations are performed on selected atoms (He, Be) and molecules (CO, C60, Be4) using all-electron or pseudo-potential formulations. 1. Davydov, D.; Young, T. & Steinmann, P. On the adaptive finite element analysis of the Kohn-Sham equations: Methods, algorithms, and implementation. International Journal for Numerical Methods in Engineering, 2016, 106, 863-888 2. Davydov, D.; Gerasimov, T.; Pelteret, J.-P. & Steinmann, P. Convergence study of the h-adaptive PUM and the hp-adaptive FEM approaches applied to PDEs in quantum mechanics. Submitted, 2017 3. Bangerth, W.; Davydov, D.; Heister, T.; Heltai, L.; Kanschat, G.; Kronbichler, M.; Maier, M.; Turcksin, B. & Wells, D. The deal.II Library, Version 8.4. Journal of Numerical Mathematics, 2016

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Title: Data-Driven Reduced-Order Modeling of Fluids Systems

Author(s): *Scott Dawson, *California Institute of Tech*; Clarence Rowley, *Princeton University*.

This talk will study methods to obtain reduced-order models and extract pertinent dynamical features for systems in fluid dynamics, using a data-driven approach. We study how finite-dimensional approximations of the Koopman operator can be utilized for the construction of accurate nonlinear reduced-order models, and investigate the performance of such models for a variety of choices of observable functions. We will compare this “ground-up” identification of dynamics from data with “top-down” projection of the full governing equations onto a low-dimensional subspace. Following this, we will explore methods by which data-driven modeling approaches can be modified to include additional system properties that may be known a priori, such as conservation laws and certain dynamical features. We will explore heuristics for how the accuracy of these methods depends on the quantity and quality of data available, and will further consider how such methods scale with the complexity of the system and dimension of the reduced-order model.

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Title: On the Algorithmic Treatment of a Constitutive Model for Mechanically-Induced Martensitic Phase Transformations

Author(s): *Daniel de Bortoli, Francisco Andrade Pires, *University of Porto*; Eduardo de Souza Neto, *Swansea University*.

In this contribution, fully implicit integration algorithms for a constitutive model for mechanically-induced martensitic transformations are proposed and analysed in terms of computational efficiency. The model studied is that developed in [1], motivated by a well-established [2] energy-based criterion for the transformation onset, generalised to multi-axial stress states and formulated in a large strain setting. It bears many similarities to classical crystal plasticity models: transformation functions (akin to yield functions) define a criterion for the martensite evolution according to preferred crystallographical directions (transformation systems). The efficient computational treatment of this type of models presents some challenges: given the large number of transformation systems (for instance, 24 in the FCC-to-BCT/BCC case), determining the subset that are active during a given time increment is not trivial. Here, two strategies are pursued and compared: a viscoplastic regularisation, and an active system selection algorithm. The former, frequently used in the crystal plasticity literature, circumvents the issue of active set determination altogether; it leads, however, to numerical difficulties when the rate-independent case is approached, in the limit of vanishing rate-sensitivity parameters. This motivates the development of strategies involving the latter approach, such as those presented in [3], applied to the rate-independent formulation. Since the constitutive model studied also includes contributions from slip plasticity in the austenitic phase – significant in some materials undergoing mechanically-induced martensitic transformations – another algorithmic question of interest concerns methods for the appropriate coupling, at the integration point level, between the relevant deformation mechanisms (slip plasticity and martensitic transformation). The proposed algorithms are presented together with their consistent linearisation. These implementations are embedded in a computational homogenisation-based multi-scale, fully implicit finite element code, where examples exploring their performance for materials of interest, such as meta-stable austenitic stainless steels, are analysed. References: [1] de Bortoli, D., 2016. Towards a Predictive Multi-Scale, Thermodynamically Consistent Constitutive Model for Mechanically-Induced Martensitic Phase Transformations. Ph.D. thesis, Swansea University. [2] Patel, J.R., Cohen, M., 1953. Criterion for the Action of Applied Stress in the Martensitic Transformation. Acta Metallurgica, 1(5), 531–538. [3] Akpama, H.K., Bettaieb, M.B., Abed-Meraim, F., 2016. Numerical Integration of Rate-Independent BCC Single Crystal Plasticity Models: Comparative Study of Two Classes of Numerical Algorithms. International Journal for Numerical Methods in Engineering, 108(5), 363–422.

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Title: From Forging to End of Lifecycle: A Multiphysics Simulation Workflow for Hydrogen Embrittlement

Author(s): *Gabriel de Frías, James Foulk III, Michael Veilleux, Kevin Manktelow, Lauren Beghini, Alexander Hanson, Andrew Stershic, Jakob Ostien, Dorian Balch, *Sandia National Laboratories*.

The rapid expansion of computational simulation capabilities over the years has enabled us to assist designers more than ever before. It is of utmost importance to understand how the subsequent manufacturing processes of forging, machining and welding will affect both mechanical properties and the residual stress state. These stages of manufacturing are unequivocally tied to the performance of the part throughout its lifecycle. In this work, we present a multiphysics simulation workflow capable of informing the design process of metallic structures by coupling various stages of the manufacturing and aging processes for qualification. We focus on particular advancements for modeling embrittled steel structures due to the presence of hydrogen over the course of several years. Using this novel workflow, we are able to realize the effects of manufacturing conditions and diverse use cases on crack driving forces and the potential onset of failure. This process relies on a wide variety of technologies to accurately model the multiphysics over an extended period of time, such as: coupled thermal, electrical, chemical and mechanical finite element codes; remeshing and remapping algorithms; and scripting to facilitate a workflow in a high performance computing environment. Through the application of the workflow to an idealized geometry, we will also touch upon the challenges of transitioning these technologies from research codes to production-ready capabilities. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: On Bounds for the Penalty Constant in Irreversibility Constraint for a Phase-Field Formulation of Brittle Fracture

Author(s): Tymofiy Gerasimov, *Laura De Lorenzis, *TU Braunschweig, Germany*.

The variational approach to fracture by Francfort and Marigo and the related regularized formulation of Bourdin et al. [1], which is also commonly referred to as a phase-field model of fracture – see the review paper [2] – is a widely accepted framework for modeling and computing the fracture failure phenomena in elastic solids. In its original mathematical ansatz, the formulation is a box-constrained minimization problem, in which a so-called crack phase-field irreversibility or, monotonicity, condition is imposed, resulting in a variational inequality system. This constrained problem can be relaxed via various penalizations as considered e.g. in [3], thus yielding an unconstrained equality-based formulation and allowing for a simpler algorithmic treatment. In our study, we focus on a formulation that involves a weakly imposed penalized irreversibility constraint, and propose an analytical procedure for estimation of an explicit lower bound for the penalty constant nested in. We deduce that this constant is, in fact, independent from a particular problem setup (geometry, boundary conditions etc.), being a function of only two generic formulation parameters such as the fracture toughness (energy release rate) and the characteristic length scale. The estimate is tested for several popular benchmarks, including those for which the exact analytical solution is available. [1] B. Bourdin, G.A. Francfort and J.-J. Marigo. The variational approach to fracture. J. Elasticity 91 (2008), 5-148. [2] M. Ambati, T. Gerasimov and L. De Lorenzis. A review on phase-field models of brittle fracture and a new fast hybrid formulation. Comput. Mech. 55 (2015), 383-405. [3] M. Artina, M. Fornasier, S. Micheletti and S. Perotto. Anisotropic mesh adaptation for crack detection in brittle materials. SIAM Journal on Scientific Computing 37 (2015), 633-659.

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Title: Modeling Force-Driven Damage in the Axon from Molecular Mechanisms

Author(s): *Rijk de Rooij, Ellen Kuhl, *Stanford University*.

An axon is a long and slender projection of a nerve cell that transmits electrical signals from the cell body to other cells. The role of mechanical forces in axon physiology was discovered several decades ago and is now widely recognized. The axon maintains a constant tension in physiological conditions, whereas external forces due to, e.g., impact on the brain may result in pathological conditions. Such pathologies are now increasingly traced back to tau-protein at the molecular level [1]. However, it is unfeasible to investigate and verify these cause-effect relationships with experiments alone. Numerical modeling provides a powerful alternative to access the interplay of key players in axonal mechanics and to bridge the molecular and axon level scales. We have recently presented a general computational framework for modeling molecular mechanisms in the axon within the context of the finite element method [2]. In this model, we assign molecular mechanisms to individual finite elements. Throughout the entire simulation, we apply these mechanisms via minor modifications to the standard Newton Raphson solver. Using our axon model—a network of microtubules connected by crosslinks—we demonstrated that our framework is capable of relating microscopic, molecular mechanisms to macroscopic axon properties including stiffness and viscosity. Here, we use our framework to investigate axonal damage caused by externally applied forces at varying loading rates. We use the phenomenological Bell model to characterize the chemical bond strength between tau-proteins and microtubules and simulate stress-strain relations of the axon up to global failure. Our results indicate that axonal damage increases with increasing strain rates, consistent with existing literature. Our model naturally bridges the scale between the molecular and continuum levels. We anticipate that molecular simulations can further inform its parameterization and that the model itself will inform constitutive models of the brain at the continuum level [3]. References [1] H. van den Bedem, E. Kuhl, Tau-ism: The Yin and Yang of Microtubule Sliding, Detachment, and Rupture. Biophysical Journal 109, 2215–2217 (2015). [2] R. de Rooij, K.E. Miller, E. Kuhl, Modeling Molecular Mechanisms in the Axon. Computational Mechanics 59(3), 523-537 (2017) [3] R. de Rooij, E. Kuhl, Constitutive Modeling of Brain Tissue: Current Perspectives. Applied Mechanics Reviews 68, 1–16 (2016)

14th U.S. National Congress on Computational Mechanics
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Title: Recent Advances in Methods with the Summation-by-Parts Property

Author(s): *David C. Del Rey Fernandez, *NASA LaRC and NIA*; David W. Zingg, Pieter D. Boom, *UTIAS*; Mark H. Carpenter, *NASA LaRC*; Jason E. Hicken, Jared Crean , *Rensselaer Polytechnic Institute*.

The solution of partial-differential equations on high-performance computing architectures necessitates flexible and robust numerical methods. The summation-by-parts (SBP) framework (see Refs. [1,3]) is advantageous in the construction of such schemes as it leads to conservative methods of arbitrary high-order that are provably linearly or non-linearly stable. Since these methods are not explicitly tied to basis functions, it is possible to tailor difference operators for different needs by optimizing the operators and/or the nodal distributions thereby providing flexibility not easily afforded by alternative discretization methodologies. For the most part, the SBP community has concentrated on tensor-product SBP operator using a traditional finite-difference approach, i.e., the operators have a repeating interior-point operator and mesh refinement is carried out by increasing the number of nodes within each block. However, the SBP concept is more broadly applicable and element based operators can be constructed and implemented using a discontinuous or continuous approach. Moreover, it is also possible to construct multi-dimensional SBP operators that are not based on tensor products (see Ref. [2]), which opens the door for discretizations on meshes tessellated with arbitrary elements. In this presentation, we summarize a number of recent developments in both tensor-product and multi-dimensional SBP methods including linear and nonlinear stability in curvilinear coordinates. [1] David C. Del Rey Fernández, Jason E. Hicken, and David W. Zingg. Review of summation-by-parts operators with simultaneous approximation terms for the numerical solution of partial differential equations. Computers & Fluids, 95(22):171–196, 2014. [2] Jason E. Hicken, David C. Del Rey Fernández, and David W. Zingg. Multi-dimensional summation-by-part operators: General theory and application to simplex elements. SIAM Journal on Scientific Computing, 4(38), 2016. [3] Magnus Svärd and Jan Nordström. Review of summation-by-parts schemes for initial-boundary-value-problems. Journal of Computational Physics, 268(1):17–38, 2014.

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Title: Reliable Modelling of Neural Network at Extreme Scale: Status, Opportunities and Challenges

Author(s): *Fabien Delalondre, *EPFL*.

The Blue Brain Project (BBP), a project at the Ecole Polytechnique Federale de Lausanne (EPFL) based in Geneva, Switzerland, aims at modelling large neural networks at three different scales on supercomputers: from point neuron, to 1D and 3D morphologically detailed neurons. Each scale which is used to address a different set of scientific questions is supported by the development and optimization of complex software executed on massively parallel machines. In order to support the optimal execution of the application software a careful performance analysis of both hardware and software must be conducted together to select the most suitable computing platform for the problems and models of interest. This recipe allows building and simulating large in-silico neural network models which prove to reproduce complex results observed in experiments for the first time, paving the way for predictive neuroscience simulation [1]. Building on concepts developed in collaboration with M. Shephard in [2], we will describe in this presentation future opportunities and challenges to reliably model the activity of neural network at extreme scale. This includes the careful estimates of errors [3] to control the accuracy and validity of the models, hardware/software co-design and performance analysis and modeling to optimally implement the needed algorithms on future hardware tailored to the application needs, the development of new components such as a source to source compiler which increases performance portability across computing platforms, the investigation of distributed mesh-based solutions to extend the set of scientific questions of interest as well as the development and application of new numerical algorithms. We hope that this presentation will spark the interest of the Computational Mechanics community in order to help build increasingly larger and more accurate models of the brain and eventually contribute to understand the most complex organ of the human body. [1] H. Markram et al., Reconstruction and Simulation of Neocortical Microcircuitry. Cell 163, 2015, 456-492. [2] F. Delalondre, C. Smith, M.S. Shephard, Collaborative software infrastructure for adaptive multiple model simulation, Computer Methods in Applied Mechanics and Engineering, Volume 199, Issues 21–22, 1 April 2010, Pages 1352–1370, http://dx.doi.org/10.1016/j.cma.2010.01.011 [3] F. Casalegno, F. Cremonesi, S. Yates, M.L. Hines, F. Schuermann, F. Delalondre, Error Analysis and Quantification in NEURON Simulations, ECCOMAS Congress 2016, Crete Island, Greece, 5–10 June 2016

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Title: Generalization of the Ordinary State Based Peridynamic Model for Isotropic Linear Viscoelasticity

Author(s): *Rolland Delorme, Ilyass Tabiai, Louis Laberge Lebel, Martin Lévesque, *Polytechnique Montreal*.

This talk aims at presenting a general peridynamic model for isotropic linear viscoelasticity that is equivalent to the classical approach. We believe that the results here are important since they provide a clear and direct means to researchers dealing with viscoelastic creep crack growth, for example, to tackle their problem within the peridynamic framework. Classical continuum mechanics is a framework that relies on partial differential equations for computing stresses and strains in a general solid submitted to external loads and boundary conditions. The spatial derivatives yield undefined stress tensors at material discontinuities. This is a well-known problem to which a number of circumventing methods have been proposed over the last century. One of them is the peridynamics framework which is a reformulation of the balance laws based on a non-local integral approach in which a material point is affected by its neighbors located within a finite distance, called the horizon. The peridynamics theory is well suited to address evolving damage problems since it completely eludes the need for spatial derivatives because it is expressed in terms of forces and displacements between material points. A generalization of the non-local ordinary state based peridynamic model for isotropic linearly viscoelastic material is proposed in this talk. This model accounts for viscoelastic spherical and deviatoric components and is based on the thermodynamically acceptable Prony series approach. The model is derived from a direct equivalence relation between the peridynamic viscoelastic parameters and the well-known creep compliance tensors used in classical viscoelasticity, by equating the free energy densities expressed in both approaches. The model is simplified to a uni-dimensional expression and implemented to simulate a quasi-static creep-recovery test. The comparison between the peridynamics and classical continuum mechanics predictions validates this implementation. An exact correspondence between peridynamics and the classical continuum approach is shown when the peridynamic horizon decreases to the mesh-size, meaning peridynamics tends toward the local approach of classical continuum mechanics.

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Title: A DPG Approach to the Full Vectorial Transverse Mode Instability Model of Optical Laser Amplifiers

Author(s): *Leszek Demkowicz, Sriram Nagaraj, *ICES, UT Austin*; Jacob Grosek, *Kirtland Air Force Base*.

In this work, we study the DPG methodology with its attractive properties of mesh independent stability, automatic adaptivity and parallelizability applied to a weakly coupled Maxwell-heat equation equation system arising in the context of laser amplification in optical fibers. The interaction of heating effects with the Maxwell system gives rise to the phenomenon of transverse mode instability (TMI). We consider the usual set of Maxwell equations with no free charges with the polarization vector including background, gain and thermal contributions. The primal DPG method is used with an implicit Euler time-stepping approach for the heat equation with radial Dirichlet conditions along the fiber. The Maxwell system is then solved with the ultraweak DPG formulation (which is known to be effective in high-frequency wave propagation problems) with polarization values obtained from the heat equation. We then iterate between the heat and Maxwell system updating the relevant quantities until convergence. The use of DPG adaptivity for the Maxwell system along with the guaranteed discrete stability of the ultraweak/primal formulations is critical for a numerically stable and tractable method which allows us to effectively simulate the TMI phenomenon.

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Title: A Novel Solver for Multi-Component/Phase Compressible Flows with Advanced Discretized Schemes on Unstructured Grids

Author(s): *Xi Deng, Bin Xie, Feng Xiao, *Tokyo Institute of Technology*; Honghui Teng, *Chinese Academy of Sciences*.

We have constructed novel numerical models for multi-component/phase compressible flow simulations on unstructured grids by employing VPM (Volume integrated average and Point value based Multi-moment) method and BVD (Boundary Variation Diminishing) principle. Different from conventional finite volume method (FVM), both the volume-integrated average (VIA) and the point values (PV) at the cell vertices are used as the computational variables updated at every time step. The VIA is computed by a finite volume formulation of flux form where the conventional Riemann problem is solved by the HLLC Riemann solver, while the PV is point-wisely updated using the differential formulation where the Roe solver is used to compute derivative Riemann problems. To suppress numerical oscillation and diffusion around discontinuities, a limiting process and a numerical diffusion minimization process have been proposed respectively base on BVD principle. In the limiting process, a smoothness indicator has been designed through which the slope limiter is in effect only around critical region. While in the numerical diffusion minimization process, the Unstructured Multi-dimensional Tangent of Hyperbola Interface Capturing (UMTHINC) formulation has been employed as one of candidates to reconstruct numerical flux. We present numerical models for two typical multi-component/phase compressible flows, i.e. interfacial five-equation model and reacting Euler equation model. Using the five-equation model, we simulated the shock-bubble interactions where the moving interfaces between two compressible flows and density perturbations are well resolved. The convergence tests demonstrate the proposed model can achieve third-order accuracy on unstructured grids for reacting Euler equations. Numerical results of detonation wave propagation benchmark tests such as the unstable oblique detonation waves (ODWs) show that the present model can produce the fine flow structures with less degree of freedoms (DOFs) in comparison with conventional FVMs that have excessive numerical dissipation and need much higher grid resolution to reproduce the flow structures. With good solution quality for multi-component/phase compressible flows on unstructured grids which can adapt complex boundaries with flexibility, the proposed models show great potential as a practical tool for numerical investigations of supersonic combustion and compressible multiphase fluid dynamics.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Anomalous Diffusion and its Applications

Author(s): *Weihua Deng, *Lanzhou University* ; Eli Barkai, *Bar Ilan University*.

Anomalous diffusion processes are wildly found in nature, including the motion of lipids on membranes, solute transport in porous media, translocation of polymers, turbulent flow, optical materials, motion of predators, human travel, etc. It is an interdisciplinary research. We will discuss the models charactering their microscopic dynamics, e.g., CTRW, Langevin picture, Levy flights, subordinated Levy processes; and derive the corresponding macroscopic descriptions, i.e., the PDEs governing the PDF of the functionals of particle trajectories or the positions of particles. The challenges of numerically solving the models will be mentioned and some physical applications will be proposed.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Temperature and Distortion Simulation for Laser Powder Bed Fusion Parts

Author(s): Pan Michaleris, *Erik Denlinger, *Autodesk Inc.*.

The warping of parts during Laser Powder Bed Fusion deposition presents a significant challenge to the process becoming an economically feasible method of component production. Component warpage frequently leads to part failure, resulting in expensive experimental trial and error iterations. This study shows that finite element modeling performed using Netfabb Simulation can be used to quickly and accurately predict the distortion of part-level components and to indicate likely failure modes, thus circumventing costly failed builds. The simulation methodology will be described and extended to cases requiring the simulation of the full build plate, including the un-melted powder and multiple parts. The effect of part interaction and placement location on the build-plate will be demonstrated for both the thermal and mechanical response. Model predictions will be compared to experimental distortion measurements.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Scalable Sampling-Free Nonlinear State Estimation Algorithm for Large-Scale Models and Data Sets using High Performance Computing

Author(s): *Ajit Desai, Philippe Bisaillon, Abhijit Sarkar, *Carleton university*; Mohammad Khalil, *Sandia National Laboratories*; Chris Pettit, *United States Naval Academy*; Dominique Poirel, *Royal Military College of Canada*.

A scalable intrusive polynomial chaos (PC) based state estimation algorithm is presented for high resolution computational models by blending large observational data sets, originating from sensor networks. For the forecast (prediction) step, the domain decomposition (DD) method based parallel interative solvers [1, 2, 3, 4] are used to efficiently propagate the polynomial chaos coefficients of the state. When sensor data is available, the PC coefficients are updated using a parallel update (analysis) step [3] of the polynomial chaos Kalman filter. Domain decomposition algorithms can provide ideal platforms to leverage high-performance computing to simulate large-scale linear system arising in the context of intrusive spectral stochastic finite element methods [1, 2, 3, 4]. The robustness and scalabilities of these solvers are enhanced by using PETSc, FEniCS and UQTk libraries. The parallel performance of these solvers are tested by concurrently tackling high resolution in spatial and stochastic dimensions. Furthermore, the preliminary investigation suggests that, with increasing stochastic dimensions, the DD based intrusive parallel solvers scale better than sampling-based (non-intrusive) sparse grid quadrature. For the update step, the DD solvers are coupled with an in-house Bayesian estimation software [3] to tackle large-scale data assimilation problems. Numerical and parallel scalabilities of the algorithm are presented for state estimation of a stationary diffusion equation having spatially varying diffusion coefficient modeled by a non-Gaussian stochastic process. References [1] W. Subber, and A. Sarkar, A domain decomposition method of stochastic PDEs: An iterative solution techniques using a two-level scalable preconditioner, Journal of Computational Physics 257 (2014): 298-317. [2] W. Subber, and A., Sarkar, Dual-Primal Domain Decomposition Method for Uncertainty Quantification, Journal of Computer Methods in Applied Mechanics and Engineering, 266 (2013), 112-124. [3] M. Khalil, Bayesian Inference for Complex and Large-scale Engineering Systems, Ph.D. thesis, Carleton University, 2013. [4] A. Desai, M. Khalil, C. Pettit, D. Poirel and A. Sarkar, Scalable Domain Decomposition Solvers for Stochastic PDEs in High Performance Computing, Computer Methods in Applied Mechanics and Engineering, 2017 (under review).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Modeling the Nucleation and Growth of Polymer Spherulites

Author(s): *Fabrice Detrez, Luc chevalier, *Université Paris-Est*.

Semicrystalline polymer materials play an essential role in the industry. The modeling and prediction of polymer microstructures has obvious environmental and economic interests. In this study, a mesoscale modeling of spherulite pattern formation is constructed. For this purpose, the spherulite growing is modeled by a multi-phase fields model and by a cellular automaton. The heterogeneous nucleation of the spherulites is modeled using the concept of random local nucleation time which allows to optimize the computational time.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: On Acoustic Scattering from Elastic Objects in the Free-Field and near a Fluid-Sediment Interface

Author(s): *Saikat Dey, *US NRL*.

Approaches to accurate simulations of three-dimensional acoustic scattering from elastic objects for several model problems are discussed. For objects in an infinite homogeneous medium, an infinite-element based approach is used to truncate the infinite exterior medium. For objects near a sediment-fluid interface two formulations are presented. The first one treats the sediment as a damped acoustic medium and the truncation of the resulting semi-finite domains is done with a so-called perfectly-matched-layer (PML) approach. In applications where the sediment must be modeled using three-dimensional linear elasticity, we identify issues of consistency when using PML with a fluid-elastic exterior domain model and present a novel alternative based on an interior-transmission approach to have a consistent method. The numerical implementation of all these formulations is based on heirarchic p-finite-element approximations. Several example problems are presented to both validate the formulations and show their practical applications.

14th U.S. National Congress on Computational Mechanics
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Title: Role of Viscosity Stratification in Tear Film Rupture

Author(s): *Mohar Dey, *University of British Columbia*; Atul Vivek, Harish Dixit, *IIT Hyderabad, India*; Ashutosh Richariya, *LVPEI Hyderabad, India*; James Feng, *University of British Columbia, Canada*.

Ocular surface disorders are one of major causes of blindness in humans due to lack of proper treatment right at its onset. We use fluid mechanical tools to understand the nature and predict the occurrence of such disorders by analyzing the break up times (BUT) of the tear film that acts as a protective cover over the sensitive corneal epithelium. The tear film is composed of three layers with very distinct rheological properties, viz., the innermost mucin layer that covers the sensitive cornea protecting it from invasive bacteria or microbes, the intermediate bulk aqueous layer that is often embedded with biopolymers in the form of soluble mucins or pathogens, and the outermost thin lipid layer which prevents evaporation and reduces the interfacial tension at the tear film-air interface. Our model takes into account the mucin distribution and its transport, the resulting viscosity profile in the aqueous layer together with the Marangoni stresses at the film/air interface and the slip effects at the base of the tear film, in an effort to understand and explain the correlation between morphological changes in the tear film and time scales of its break up. This is accomplished by carrying out a detailed linear stability analysis along with a non-linear study to determine the rupture times and also to probe the role of various components of the pre-corneal tear film in the dynamics of rupture. References R. J. Braun, Annu. Rev. Fluid Mech. 44, 267-97 (2012).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Coupled Moisture Diffusion and Mechanical Analysis to Evaluate the Differential Drying of Concrete: Application to Failure Prediction of Concrete Material

Author(s): *Razakamandimby Ranjanoro Diamondra Fenosoa Tiana, .

Drying of composite material such as concrete leads to the reduction of the volume and induces micro-cracks (failure). This drying does not occur uniformly since it starts from the material surface to the ambient environment. And due to the effect of aggregate which has different material properties, volume change can be restrained. This complexity of the drying makes the prediction of failure difficult. To overcome the problem, it is presented in this paper an application of the coupled moisture diffusion and mechanical analysis to model the differential drying of concrete and predict the failure. By solving the nonlinear coupled equations, using an exact implementation of Newton's method, the tensile stress at each given time and location within the domain can be evaluated. When the tensile stress exceeds the admissible tensile stress, the cracks will be initiated at that point and that time. An application to the drying of concrete with different aggregate volume fraction was performed to validate the accuracy of the coupling method. Results shows the initiation of cracks that occurs on the surface or on the interface of aggregate and cement paste due to high stress induced by difference in material properties. References: 1) J.-K. Kim, C.-S. Lee "Prediction of differential drying shrinkage in concrete", Received 3 April 1997, Accepted 12 May 1998, Available online 15 November 1998 2) Weiss, W. J. Yang, W., and Shah, S.P. (1998), "Shrinkage cracking of restrained Concrete Slabs", ASCE journal of Engineering Mechanics, Vol. 124, Np. 7, PP765-774

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Topology Optimization Scheme to Distribute Lattice Infill in Additive Manufacturing

Author(s): Francesco Campagna, *Politecnico di Torino*; *Alejandro R Diaz, *Michigan State University*.

We consider a problem in design of structural components for additive manufacturing. The work focuses on load-bearing components whose outside shape is fixed, determined by a “skin”, typically a relatively thin layer of material. The design space is the volume inside this skin, where the goal is to design reinforcement that stiffens the part. Reinforcement is lattice material of prescribed topology. Within the design domain, internal boundaries of solid material are designed to separate regions of lattice material of the same microstructural scale. This scale may vary from region to region in the domain. The goal is to find distributions of the lattice that maximize structural stiffness. The method is based on a topology optimization scheme to position internal boundaries separating lattice regions, and relies on effective properties of known lattice topologies. The method has been described for extruded 3D geometries loaded in-plane. Boundaries separating regions of similar scale lattices are positioned using a standard topology optimization problem using a density approach and a SIMP model. Regions assigned high effective density become the walls that separate regions filled by lattice. Closed sub-domains Ωi separated by solid material are identified through image processing. Each Ωi is candidate for lattice infill with lattice parameters that are constant within each Ωi but can vary from one sub-domain to another. In a second analysis stage, material in each Ωi is assigned effective properties Di = f(di) D0i. Di is an elastic tensor whose properties correspond to the effective properties of a known (periodic) lattice. f(di) is a scaling parameter that depends on the effective density of the lattice, di , and of the lattice topology. The second optimization problem assigns optimal values to the dis. While at this stage several possible objective functions can be considered (e.g., local buckling, thermal energy dissipation, vibration absorption) we again consider stiffness as the driving criterion at this stage. Using effective properties here decouples the underlying finite element mesh from the lattice geometry and allows the use of lattices of scales independent of the finite element size. The characteristic length (L) of the lattice used within each subdomain and the thickness (t) of each lattice member are obtained via and inverse problem that maps each effective density d to lattice parameters (L and t). The final step involves the generation of information suitable for 3D printing and the actual printing of the part, e.g., a standard STL file.

14th U.S. National Congress on Computational Mechanics
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Title: Molecular Dynamics Based Predictive Modeling of High Strain Rate Fragmentation in Metals

Author(s): *Doyl Dickel, Bradley Huddleston, Mark Horstemeyer, *Mississippi State University*.

Continuum level models of fragmentation in metals are capable of providing general trends for the size and energy of fragments based on the strain rate and strength of the material fragmenting. However, the underlying microstructure and history of the material are rarely considered as part of these models. Using molecular dynamics simulations of catastrophic fragmentation, we demonstrate a fundamental relationship between the nucleation and presence of defects in nano-crystalline copper and the eventual fragment sizes into which it will break. These quantifiable values are then used to augment an existing finite-element damage model to give statistical predictions on the fragmentation of real materials under various impacts scenarios. We further explore how atomistic models can provide valuable insights into the onset of fragmentation and the properties of the resulting fragments.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Experimental Validation of Elastic State-Based Peridynamic for PMMA and Epoxy Materials

Author(s): *Patrick Diehl, Ilyass Tabiai, Martin Levesque Levesque, *Polytechnique Montreal*.

First, we use the displacement extracted from the experiment via digital image correlation to compute the peridynamic state-based force tensors. Now the elastic properties of each material can be compared with the ones obtained for each material in the experiment. Second, a peridynamic simulation is done using the Young Modulus and Poisson's ratio extracted from the experiment. Here, we compare the displacement obtained in the simulations with the respective ones from the experiment. Thus, we can validate if the peridynamic force tensor corresponds to the measured Young's modulus in the experiment. In addition, we can verify the displacement field from the experiment with the obtained one in the simulations. After the verification and adjustment of the material parameters, more complex tensile tests with inclusions of fibers could be considered.

14th U.S. National Congress on Computational Mechanics
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Title: Using Hyper-Dual Numbers to Integrate an Equation of State into a Phase Field Model for Droplets

Author(s): *Felix Diewald, Charlotte Kuhn, Michaela Heier, Hans Hasse, Ralf Müller, *University of Kaiserslautern*; Martin Horsch, *Indian Institute of Technology Kanpur*; Kai Langenbach, *Rice University*.

Many production processes demand predictions of the wettability of structured component surfaces. Molecular dynamics (MD) simulations are capable of predicting wetting phenomena accurately [1] but are limited to nanoscopic length scales. The presented finite element phase field model aims to transfer the insights of the MD simulations to larger computational domains. To do so, the free energy of the system is defined by an equation of state that corresponds to the force field used in the MD simulations. This approach ensures consistency between the MD and the phase field simulations and leads to an interpretation of the order parameter of the phase field model as the local density (liquid/gas). Physical phenomena like temperature dependence of the bulk densities or interface width can be reproduced by the model. For the weak form of the free energy as well as the tangent of Newton's method, first and second derivatives with respect to the local density are required. The high complexity of the equation of state makes its explicit derivation time consuming and prone to errors. By using hyper-dual numbers an easy and fast implementation as well as interchangeability between different equations of states becomes possible. Extending the advantages of a complex step first derivative approximation, hyper-dual numbers allow to calculate exact and step-size independent first and second derivatives [2]. A detailed discussion of the finite element implementation which uses operator overloading to extend mathematical operations to the new variable class of hyper-dual numbers will be followed by illustrative examples that demonstrate the pertinency of the approach. References [1] S. Becker, H.M. Urbassek, M. Horsch, H. Hasse: Contact Angle of Sessile Drops in Lennard-Jones Systems, Langmuir, 30(45), 13606-13614 (2014). [2] J.A. Fike, J.J. Alonso: The Development of Hyper-Dual Numbers for Exact Second-Derivative Calculations, In AIAA paper 2011-886, 49th AIAA Aerospace Sciences Meeting (2011).

14th U.S. National Congress on Computational Mechanics
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Title: High-Dimensional Separable Compression and Basic Operations: A PGD Arithmetic Toolbox

Author(s): *Pedro Diez, Sergio Zlotnik, Antonio Huerta, *UPC-BarcelonaTech*.

Separable approximations efficiently deal with high-dimensional data. In particular, the Proper Generalized Decomposition (PGD) provides separable functions as solutions of boundary value problems. The general PGD framework contains a large family of methodologies, all of them providing solutions of separable objects, that is a sum of terms, being each term a product of 1D functions (or arrays). Some of the PGD methodologies have been conceived to tackle nonlinear problems. We present a general methodology to perform basic operations (sum, product, division, exponentiation...) for this type of objects. The idea is based on the principle of PGD compression, which is a separable least squares approximation of any multidimensional function. The PGD compression is extensively used in practice to compact the separable solution in few terms without loss of accuracy. Here, this concept is applied to both algebraic tensor structures and functions in multidimensional Cartesian domains. Moreover, a straightforward extension of this concept is devised to operate with multidimensional objects stored in the separable format. That allows creating a toolbox of PGD arithmetic operators. Thus, the toolbox is used to perform elemental operations with PGD type objects. This is of particular interest to solve nonlinear problems with PGD techniques by simply replicating the iterative algebraic solvers that are used in the standard Finite Element framework.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: The Moving Porous Green's Function Associated with Doppler's Effect in BEM and Analysis for Vehicle Jumping on Highways

Author(s): *B.Y. Ding, Y. Z. Song, *Zhejiang University City College*.

Based on the Betti-Rayleigh reciprocal theorem and the principle of relative moving, the Green's functions subjected to a moving load associated with Doppler's effect are presented. The appropriate forms of expression for moving Green's functions are suggested in u-p formulation. Using the solution decoupling of the dilational waves in Biot's dynamic equation, the responses of the displacement, the porous pressure and drainage in frequency domain have numerically been implemented in BEM via Somigliana's and Volterra's representations, respectively. The results reveal that: affected by Doppler's effect, the porous pressure exists some differential causing drainage in subgrade of the saturated soft silt. Such drainage can lead to subsidence of bridge pier on highways, and subsidence in the pier where takes place the vehicle moving away from is more serious than that moving toward■which make vehicles jump after passing bridges. It is the so-called "vehicle jumping" in traffic engineering, which frequently causes accidents. Because vehicle jumping has never been analyzed and evaluated so far, in this paper, the authors analyze the existing engineering data to verify theory and to improve the design methodology. Authors also believe relevant investigation in this paper will be useful for design and can be helpful to reduce the number of accidents. Key words: the moving porous Green's function; the Doppler's effect; the vehicle jumping; BEM. Authors acknowledge financial support from the NSFC (National Natural Science Foundation of China) (No.51478435, 11172268). References: [1] Theodorakopoulos DD. Dynamic analysis of a poroelastic half-plane soil medium under moving loads. Soil Dynamics and Earthquake Engineering 2003; 23(7): 521-533. [2] Beskou ND, Tsinopoulos SV, Theodorakopoulos DD. Dynamic elastic analysis of 3-D flexible pavements under moving vehicles: A unified FEM treatment. Soil Dynamics and Earthquake Engineering 2016; 82: 63-72. [3] Cheng AHD, Detournay E. On singular integral equations and fundamental solutions of Poroelasticity. International Journal of Solids and Structures 1998;35(34-35):4521-4555. [4] Ding BY, Yuan JH. Dynamic Green's functions of a two-phase saturated medium subjected to concentrated force. International Journal of Solids and Structures 2011; 48: 2288-2303. [5] Ding BY, Cheng AHD, Chen ZL. Fundamental solutions of poroelastodynamics in frequency domain based on wave decomposition. Journal of Applied Mechanics2013;80:6021-6012. [6] Cao YM, Xia H, Lombaert G. Solution of moving-load-induced soil vibrations based on the Betti–Rayleigh Dynamic Reciprocal Theorem. Soil Dynamics and Earthquake Engineering 2010; 30(6): 470-480. [7] Ding BY, Jing JQ, Hu J. The treatment of BEM for porodynamic problems subjected to a force source in time-domain. Engineering Analysis with Boundary Elements 2016; 67: 138-151.

14th U.S. National Congress on Computational Mechanics
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Title: Computational Simulations of Tertiary Blast Emphasize the Need for Blunt Impact Protection

Author(s): *Jean-Philippe Dionne, Aris Makris, Jeffrey Levine, *Med-Eng*.

Explosive Ordnance Disposal (EOD) ensembles (bomb suits) provide protection against the main threats of blast: overpressure, fragmentation, impact and heat. While emphasis is often put on fragmentation and overpressure (including computational studies), the present paper focuses on impact (tertiary) injuries and the relevance of bomb suit blunt impact protection. When exposed to blast, EOD technicians are likely to be launched by the strength of the blast wave, thereby hitting surrounding obstacles, hence the need for impact protection. The launch distance, or displacement of the center of gravity of the operator, is an empirical indication of explosive event severity. The velocity at which the technician hits obstacles depends largely on the amount of explosive, the initial standoff distance, and orientation. In a previous study, a simple analytical model had been devised based on experimental observations of dressed mannequins and human surrogates subjected to blast, to estimate the launched distance for free-field scenarios, based on explosive mass and standoff. Unfortunately, the simple analytical model relied on many simplifying assumptions. To address this gap, the present paper introduces numerical simulations (LS DYNA) using the Hybrid III mannequin model, exposed to various blast configurations and considers the bomb suit mass, to estimate impact velocities and thereby estimate potential for impact injuries. The LS DYNA model also provides an indication of the “falling mode”, i.e. the position of the mannequin as it hits the ground. Numerical simulations confirmed the experimental observations that EOD technicians can be propelled at large velocities, thereby requiring a high level of blunt impact protection (mostly for the head and spine). Additional numerical simulations simulated actual real-life events, by mimicking body displacement, towards forensics applications. The present study emphasizes that bomb suits must provide blunt impact injury protection in addition to overpressure and fragmentation protection, to optimize survivability levels, based on the fact that blast events that are deemed survivable from a direct impact with the blast were found to result in large global displacements and corresponding ground impact velocities. EOD helmets must therefore be equipped with padding or other systems to provide head impact attenuation, and bomb suits should be equipped with effective spine protectors to mitigate impacts to the delicate spinal column area. The threat of tertiary blast injuries is real and potentially severe. While the focus of this paper was on EOD operations, the main findings also apply to dismounted soldiers not involved in EOD work.

14th U.S. National Congress on Computational Mechanics
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Title: Efficient Moving Mesh Methods for Fourth Order Partial Differential Equations: Modeling Electrostatic Deflections.

Author(s): *Kelsey DiPietro, Alan Lindsay , *University of Notre Dame*.

We develop a robust moving mesh finite difference method for the simulation of fourth order nonlinear PDEs describing elastic-electrostatic interactions in two dimensions. We use and extend the r-adaptive methods developed by [1] to solve two fourth order PDEs with different evolutionary dynamics. The first PDE displays finite time quenching singularities that form at discrete spatial location(s). In this case, the moving mesh method must detect temporally forming singularities and dynamically resolve them to proper length scales. The second PDE is a regularized model which considers the elastic-electrostatic interactions that occur after the quenching singularity occurs. The solution to this PDE has initial curved interface that propagates through the domain until it is pinned at the boundaries. Unlike the quenching case, the interface location and curvature characteristics are known at the beginning of the simulation, so the role of the moving mesh method is to dynamically shift mesh points to track the interface and to accommodate for its growing perimeter. This problem is particularly challenging since asymptotic analysis shows the presence of multiple boundary layers evolving at different time scales. We accurately resolve these challenging boundary layers by integrating the asymptotic behavior into the moving mesh PDE, resulting in greater resolution near all the boundary layers. The method utilizes the self-similar and boundary layer structures of the two PDES to locate and dynamically resolve the desired properties of each equation to high accuracy. We compare our numerical approximation to the asymptotic approximations of the solutions developed in [2,3]. The presented work is the among the first to use moving mesh methods on a fourth order problem and can resolve to high accuracy with limited computational costs. In addition, it develops a framework for using asymptotic solutions to guide adaptive algorithms. References: [1] C.J. Budd and J.F. Williams. Moving mesh generation using the parabolic monge-ampere equation.SIAM Journal on Scientific Computing, 31(5):3438-3465, 2009. [2] A.E. Lindsay and J. Lega, Multiple quenching solutions of a fourth order parabolic PDE with a singular nonlinearity modeling a MEMS capacitor.SIAM Journal On Applied Mathematics, 72(3):935-958, 2012. [3] A.E. Lindsay, J. Lega, K.B. Glasner. Regularized model of post-touchdown configurations in electrostatic mems: interface dynamics. IMA Journal of Applied Mathematics, 80(6):1635-1663, 2015.

14th U.S. National Congress on Computational Mechanics
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Title: Recent Advances in Spline-Based Embedded Finite Element Methods

Author(s): Yingjie Liu, *John Dolbow, *Duke University*; Wen Jiang, *Idaho National Laboratory*.

We discuss several recent advances in spline-based embedded finite element methods. We focus attention on interface problems in which Nitsche-based approaches are used to enforce interfacial constraints. We describe the use of hierarchical local refinement methods to improve the geometrical representation of curved interfaces, as well as novel weighting methods for the interfacial consistency terms. To address small cut cells, we rely on ghost-penalty type stabilization methods. The effect of the ghost penalty terms is studied with numerical analysis and verified using several numerical examples. Several numerical results are also provided to demonstrate the accuracy and robustness of the methods.

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Title: A Mixed Finite Element Method for the Muscle-Tendon-Aponeurosis Complex

Author(s): *Sebastian Dominguez, Nilima Nigam, *Simon Fraser University*.

The mechanical response of the muscle-tendon unit to activation and external forcing depends on architectural details, activation patterns as well as the details of soft-tissue properties. In this talk we will describe the (highly nonlinear) elastic equations governing this response for a fully three-dimensional, quasi-static, fully nonlinear and anisotropic MTU. We describe a three-field mixed formulation for this problem, and present a DG discretization strategy. The scheme was implemented using {\tt■ ■deal.ii}. We present computational results about the effects of localized activation, the effects of intramuscular fat, as well as fibre curvature. This is joint with Hadi Rahemi, David Ryan and James Wakeling.

14th U.S. National Congress on Computational Mechanics
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Title: Adaptive Mesh Refinement and Domain Decomposition in Elasticity Imaging

Author(s): *Li Dong, Nicholas Hugenberg, Dhruv Patel, Assad Oberai, *Rensselaer Polytechnic Institute*; Tom Seidl, *Sandia National Laboratories*; Paul Barbone, *Boston University*.

Material properties of soft tissues, such as the Young's modulus and nonlinear elastic parameters, can be inferred by solving an inverse problem given the quasi-static tissue deformation data. This inverse problem is often posed as an optimization problem constrained by the PDEs that describe the balance of linear momentum [1]. This optimization problem can be solved efficiently using gradient-based optimization methods coupled with adjoint-equations and material continuation strategies [2]. Recent advances in ultrasound and optical coherence tomography have led to high-resolution three-dimensional displacement data that is measured on grids with several million points. This volume of data challenges the techniques discussed above. In this talk we will describe how adaptive grid refinement and domain decomposition methods may be used to address this challenge. In particular, adaptive grid refinement allows us to focus the computational effort to regions where it is most needed, while the use of domain decomposition techniques allows the parallel solution of this problem with minimal communication. We demonstrate the usefulness of these techniques on synthetic and clinical data. [1] Oberai, A. A., Gokhale, N. H., & Feijóo, G. R. (2003). Solution of inverse problems in elasticity imaging using the adjoint method. Inverse problems, 19(2), 297. [2] Oberai, A. A., Gokhale, N. H., Goenezen, S., Barbone, P. E., Hall, T. J., Sommer, A. M., & Jiang, J. (2009). Linear and nonlinear elasticity imaging of soft tissue in vivo: demonstration of feasibility. Physics in medicine and biology, 54(5), 1191.

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Title: Hydraulic Fracture's Near Tip Behavior: Effects of Fluid Rheology, Turbulence, Stress Variation, and Proppant

Author(s): *Egor Dontsov, *University of Houston*.

Near tip behavior of a hydraulic fracture plays an important role in understanding the global fracture behavior. From mathematical perspective, the near-tip solution is equivalent to that for the problem of a semi-infinite hydraulic fracture that propagates steadily under plane strain elastic conditions. Even such a simple problem is known to obey a complex multiscale behavior due to an interplay between the viscous forces, fracture toughness, and leak-off. This talk presents an approach to obtain an efficient numerical solution for the problem, which is based on the so-called non-singular formulation. This formulation eliminates singular pressure from the unknowns and enables one to use standard numerical techniques to obtain the result. Several problems are addressed using this approach. All of them consider the tip region problem in the presence of viscous fluid flow (Newtonian or power law), fracture toughness, Carter leak-off, and some other features as applicable. In particular, these problems can be summarized as: i) semi-infinite hydraulic fracture driven by a Newtonian fluid; ii) semi-infinite hydraulic fracture driven by a power law fluid; iii) semi-infinite hydraulic fracture driven by a laminar-to-turbulent flow of a Newtonian fluid; iv) semi-infinite hydraulic fracture with the presence of stress variation; v) semi-infinite hydraulic fracture with proppant; and vi) semi-infinite hydraulic fracture with the presence stress gradient (buoyancy driven hydraulic fracture). Numerical solutions to all these problems allow one to better understand the effect of a particular physical process on a hydraulic fracture's behavior. In addition, closed form approximate solutions for the problems i) and ii) are obtained. These solutions provide a result virtually instantly and are used in the Implicit Level Set Algorithm to effectively incorporate the multiscale near-tip behavior into the numerical solution. In addition, these near-tip solutions are used to develop approximations for the problems of a radial and plane strain hydraulic fracture, which capture all the regimes of propagation (storage viscosity, storage toughness, leak-off viscosity, and leak-off toughness) and all transitions between them. Approximate solutions for problems iii)-vi) are not yet obtained, but the numerical solution of the problem iv) is used as a propagation condition for the problem of a plane strain hydraulic fracture propagating in a finely stress-layered rock. The use of such a solution, that captures the fine-scale stress variation in the tip element, permits one to use the element size that is larger than the layer thickness and achieve a better computational efficiency.

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Title: Hydraulic Fracture's Near Tip Behavior: Effects of Fluid Rheology, Turbulence, Stress Variation, and Proppant

Author(s): *Egor Dontsov, *University of Houston*.

Near tip behavior of a hydraulic fracture plays an important role in understanding the global fracture behavior. From mathematical perspective, the near-tip solution is equivalent to that for the problem of a semi-infinite hydraulic fracture that propagates steadily under plane strain elastic conditions. Even such a simple problem is known to obey a complex multiscale behavior due to an interplay between the viscous forces, fracture toughness, and leak-off. This talk presents an approach to obtain an efficient numerical solution for the problem, which is based on the so-called non-singular formulation. This formulation eliminates singular pressure from the unknowns and enables one to use standard numerical techniques to obtain the result. Several problems are addressed using this approach. All of them consider the tip region problem in the presence of viscous fluid flow (Newtonian or power law), fracture toughness, Carter leak-off, and some other features as applicable. In particular, these problems can be summarized as: i) semi-infinite hydraulic fracture driven by a Newtonian fluid; ii) semi-infinite hydraulic fracture driven by a power law fluid; iii) semi-infinite hydraulic fracture driven by a laminar-to-turbulent flow of a Newtonian fluid; iv) semi-infinite hydraulic fracture with the presence of stress variation; v) semi-infinite hydraulic fracture with proppant; and vi) semi-infinite hydraulic fracture with the presence stress gradient (buoyancy driven hydraulic fracture). Numerical solutions to all these problems allow one to better understand the effect of a particular physical process on a hydraulic fracture's behavior. In addition, closed form approximate solutions for the problems i) and ii) are obtained. These solutions provide a result virtually instantly and are used in the Implicit Level Set Algorithm to effectively incorporate the multiscale near-tip behavior into the numerical solution. In addition, these near-tip solutions are used to develop approximations for the problems of a radial and plane strain hydraulic fracture, which capture all the regimes of propagation (storage viscosity, storage toughness, leak-off viscosity, and leak-off toughness) and all transitions between them. Approximate solutions for problems iii)-vi) are not yet obtained, but the numerical solution of the problem iv) is used as a propagation condition for the problem of a plane strain hydraulic fracture propagating in a finely stress-layered rock. The use of such a solution, that captures the fine-scale stress variation in the tip element, permits one to use the element size that is larger than the layer thickness and achieve a better computational efficiency.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Bi-Fidelity, Low-Rank Approximation Technique for Uncertainty Quantification

Author(s): *Alireza Doostan, Hillary Fairbanks, Jerrad Hampton, *CU Boulder*; Akil Narayan, *University of Utah*.

The use of model reduction has become widespread as a means to reduce computational cost for uncertainty quantification of PDE systems. In this work, we present a model reduction technique that exploits the low-rank structure of the solution of interest, when exists, for fast propagation of high-dimensional uncertainties. To construct this low-rank approximation, the proposed method utilizes models with lower fidelities (hence cheaper to simulate) than the intended high-fidelity model. After obtaining realizations to the lower fidelity models, a set of reduced basis and an interpolation rule are identified and applied to a small set of high-fidelity realizations to obtain this low-rank, bi-fidelity approximation. In addition to the construction of this bi-fidelity approximation, we present convergence analysis and numerical results.

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14th U.S. National Congress on Computational Mechanics
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Title: A Systematic Study of Swelling-Induced Instabilities of Hydrogels

Author(s): *Berkin Dortdivanlioglu, Andreas Krischok, Christian Linder, *Stanford University*; Ali Javili, *Bilkent University*.

Various surface instabilities such as creases and wrinkles are observed in confined hydrogels. Instabilities are triggered by the increase in compressive stresses within the hydrogel due to swelling in the presence of mechanical constraints. In general, swelling is caused by the intake and diffusion of solvent neighboring the hydrogel. When compressive stresses due to swelling reach a critical point, surface instabilities emerge. Applications of hydrogels with controlled surface instabilities range from sensors, to responsive coating and bioadhesives. Numerical models for hydrogels require coupling the deformation of the solid matrix and the diffusion of the solvent (water). Here, we adopt a mixed variational formulation of a saddle point principle with displacement and chemical potentials fields. Due to the incompressibility constraints, simulations suffer from (spurious) numerical oscillations in the nodal chemical potential solution; the formulation fails to satisfy the Ladyzhenskaya-Babuska-Brezzi (LBB) condition. A stable discretization based on isogeometric analysis (IGA) and subdivision property of B-splines is adopted to obtain oscillation-free solution fields, satisfying the LBB condition. Equipped with a robust framework for hydrogels, eigenvalue analysis can accurately capture the onset and pattern of wrinkling instabilities [1]. A perturbation technique is further required to study the post-instability response [2]. The objective of this presentation is to establish a computational framework to capture the swelling-induced instabilities of hydrogels. Furthermore, this study systematically provides phase diagrams investigating the influence of the thickness of hydrogel layers and the material properties of both the polymer network and solvent, thereby predicting the surface patterns and the onset of instabilities. Our proposed framework allows a better understanding of pattern formation in hydrogels as well as structurally similar biological tissues, and consequently promote novel engineering and biomedical applications. References: [1] Javili, B. Dortdivanlioglu, E. Kuhl, and C. Linder (2015), Computational aspects of growth-induced instabilities through eigenvalue analysis. Computational Mechanics, 56(3):405-420. [2] Dortdivanlioglu, A. Javili, and C. Linder (2017), Computational aspects of morphological instabilities using isogeometric analysis. Computer Methods in Applied Mechanics and Engineering, 316:261-279.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Minimum Required Spatial Resolution for Image-Based Simulations of Mitral Valve

Author(s): *Andrew Drach, Amir Khalighi, Michael Sacks, *University of Texas at Austin*.

Multiple studies have demonstrated that the geometries unique to each patient can affect the durability of mitral valve (MV) repairs. While computational modeling of the MV is a promising approach to improve the surgical outcomes, the geometrically complex structure of the MV presents significant challenges in the development of patient-specific computational models. We thus developed a novel pipeline for building detailed high-fidelity attribute-rich computational models of MV from in-vitro imaging data. The approach combines geometric information from loaded and unloaded states to achieve a high level of anatomic detail, followed by the mapping and parametric embedding of tissue attributes to build an attribute-rich computational model. The resulting MV model further provides the flexibility in the selection of level of detail, independent of the level of discretization. We illustrate the methodology by building the ovine MV model from in-vitro micro-CT imaging data of the normal physiological state. The predictions for displacements and surface strains are compared to the values extracted from the imaging data. We demonstrate the effect of changing the levels of details and discretization on the simulation predictions, and estimate the required level of fidelity for building predictive models. We conclude that the proposed approach enables robust biomechanical simulations of MV under different physiological states.

14th U.S. National Congress on Computational Mechanics
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Title: A Revised Tangle-Free Algorithm for Two-Dimensional Mesh Motion Problems

Author(s): *Justin Droba, Adam Amar, *NASA Johnson Space Center*.

Problems with computational domains that change with the evolution of time arise naturally in numerical simulations involving ablation, the process by which extreme heating conditions induce a material to jettison mass through thermal and chemical processes such as (but not limited to) sublimation and oxidation to reduce internal conduction and dissipate energy. Mesh motion algorithms, not to be confused with moving-mesh schemes for adaptive grid redistribution, power the modeling of these evolving grids. In previous work, we introduced the tangle-free scheme, a set of context-based boundary conditions (directions of motion) that can accommodate intense mesh deformation and enable responsive motion ("sliding") along arbitrary surfaces. Node-based penalty-method enforcement, formulated previously, of these conditions scales poorly with problem size and leads to ill-conditioned linear systems. The revised two-dimensional tangle-free algorithm to be presented here instead weakly-enforces the boundary conditions via integral formulation. However, this necessitates an overhaul of the previously developed sliding conditions: now, rather than be partially determined by system dynamics, updates to sliding nodes are wholly computed a priori by means of a one-dimensional shadow grid. This innovation also powers a significant improvement in the handling of receding surfaces adjacent to other receders. The direction of motion for nodes on these double receders is obtained by constructing a virtual sliding surface and resolving its motion. This presentation will highlight these new developments in mesh motion and demonstrate their effectiveness on contrived problems as well as real-world examples relevant to spacecraft thermal protection systems.

14th U.S. National Congress on Computational Mechanics
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Title: Robust Topology Optimization under Loading Uncertainty Using a Density Matching Approach

Author(s): *Bingxiao Du, Yong Zhao, Wen Yao, Xiaoqian Chen, *NUDT*; Timoleon Kipouros, Geoff Parks, *University of Cambridge*.

Uncertainty is important to include during design and optimisation to produce structures that are reliable and robust. The robust topology optimization under loading uncertainty is considered in this paper. Loading magnitude and direction uncertainty is introduced into the minimization of compliance problem. Since most topology optimization algorithm requires first-order gradient, a density matching approach is used to provide an objective decreasing direction for the optimization under uncertainties. Instead of giving a safety bound, the mean value and the variance of the structural performance are treated as two objectives to provide the designer with a set of Pareto optimal solutions. Numerical results on Messerschmitt–Bolkow–Blohm beams and cantilever beams in 2D demonstrate the effectiveness of the proposed formulations.

14th U.S. National Congress on Computational Mechanics
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Title: A Scale-Bridging Generalized Finite Element Method for Parallel Simulations of Spot Welds in Large Structures

Author(s): *Armando Duarte, Haoyang Li, *University of Illinois at U-C*.

Spot welds are commonly used to join thin gauge metallic structural components of automotive and aerospace vehicles. The stiffness of these components is strongly dependent on the design of their sub-component connections. Multi-point constraints are commonly used to represent spot welds in finite element models. However, they lead to mesh-dependent solutions and provide no useful information about the stresses around the spot weld, which are needed for life prediction of the connection. In this talk, we present a Generalized Finite Element Method (GFEM) based on the solution of interdependent macro/global and fine/local scale problems. The local problems focus on the resolution of fine-scale features of the solution near regions with singularities or localized nonlinearities, while the global problem addresses the macro-scale behavior of the structure. Fine-scale solutions are accurately computed in parallel using the h-version of the GFEM and embedded into the global solution space using the partition of unity method. Thus, the proposed method does not rely on a-priori knowledge about the solution of the problem. This GFEM enables accurate modeling of problems involving nonlinear, multi-scale phenomena on macro-scale meshes that are orders of magnitude coarser than those required by the FEM. Numerical examples demonstrate applications to the analysis of structural connections (spot welds) in built-up panels for the next-generation hypersonic aircrafts currently under investigation at U.S. Air Force Research Laboratories. They also show that the conditioning of the method is of the same order as in the FEM and that it is controlled by the mesh size of the coarse scale discretization.

14th U.S. National Congress on Computational Mechanics
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Title: Different Flavors of Adaptive Mesh Refinement Use in FLASH

Author(s): *Anshu Dubey, *Argonne National Laboratory*.

FLASH is a multiphysics adaptive mesh refinement (AMR) code used by several science and engineering domains, including high-energy density physics, astrophysics, cosmology, solar physics, laser plasma, and computational fluid dynamics. Most FLASH applications rely on AMR, however, each domain has its own quirks and constraints that cause a wide variation in how they use AMR. Additionally, they all use the available infrastructure and capabilities of the code in different ways. In this presentation I will give specific examples of customized utilization of FLASH AMR by various domains, while also highlighting the design aspects of the code that make it possible. I will conclude with future developments to expand the reach of these capabilities to wider communities.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Stochastic Upscaling of Elastic and Damage Behavior of Concrete at Mesoscale

Author(s): *Vasav Dubey, *Texas A&M University*; Arash Noshadravan, *Texas A&M University, College Station*.

The elastic and damage behavior of concrete is strongly influenced by the characteristics of its highly heterogeneous microstructures, such as volume fractions and parameters defining the spatial distribution and mechanical properties of its subscale constituents. The mesoscale structure of concrete is best described by three phases consisting aggregates (inclusion) in cement paste (matrix), and interfacial transition zone (ITZ), a thin high porosity zone surrounding aggregates. Uncertainty exists in composition and mechanical properties of these constituents, which in turn causes spatial heterogeneity in the local material behavior. The existing homogenization schemes are often based on idealized descriptions of micro-heterogeneities and as such they do not take into account the randomness in the morphological features. In this research we present a stochastic upscaling of mechanical behavior of concrete microstructure. We first present a statistical model for generating random microstructures that are consistent with available morphological measurements in a prescribed statistical sense. These morphological features include local aggregate volume fraction, size and shape of aggregate, spatial measurement parameter (nearest neighbor distance), thickness of ITZ and mechanical properties of ITZ. A stochastic computational homogenization, using the Monte Carlo simulation, is performed on random microstructures to characterize the micromechanics-based bounds on apparent elasticity tensor associated with the mesoscale volume elements. An upscaling methodology based on the theory of micromechanics, random matrix theory and maximum entropy principle is adopted to construct an efficient probabilistic model for elastic apparent properties of concrete microstructure at the mesoscale. The results of calibrated model are compared and validated, in a statistical sense against analytical homogenization approximations as well as finite element based numerical homogenization. Furthermore, we use similar framework to construct a stochastic description of damage behavior in at mesoscale. To that end an isotropic progressive damage model is introduced at microscale to capture damage behavior of concrete. Using finite element method we will generate requisite information for upscaling damage behavior of concrete at mesoscale. This upscaling procedure provides a computationally efficient material description that can be used for macroscale simulation taking into account local fluctuations that are connected to the subscale microstructural features. References: J. Guilleminot, A. Noshadravan, C. Soize, R.G. Ghanem, A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures, 2011 P. Wriggers, S.O. Moftah, Mesoscale models for concrete: Homogenisation and damage behaviour, 2006

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Paradigm for Predictive Modeling of Computational Mechanics Using Field Inversion and Machine Learning

Author(s): *Karthik Duraisamy, *Univ of Michigan*.

The pursuit of accurate predictive models is a central issue and pacing item in computational mechanics. With the recent growth in computational power and measurement resolution, there is an unprecedented opportunity to use data from fine-scale simulations, as well as critical experiments, to inform, and in some cases even define predictive models. While the general idea of data-driven modeling appears intuitive, the process of obtaining useful predictive models from data is less straightforward. A coordinated approach of experimental design, statistical inference and machine learning is required. Field inversion is used to obtain spatio-temporally distributed functional terms that directly address discrepancies in the structural form of the model. Once the inference has been performed over a number of problems that are representative of the underlying physics, machine learning techniques are used to reconstruct the functional corrections in terms of features that appear in the closure model. When the machine learning-generated model forms are embedded within a standard solver setting, we show that much improved predictions can be achieved, even in geometries and flow conditions that were not used in model training. The usage of very limited data as an input to construct comprehensive model corrections provides a renewed perspective towards the use of sparse amounts of available experimental datasets towards the end of developing predictive models. Examples from turbulence, combustion and materials physics will be highlighted.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Modeling the Blast Resistance of Reinforced Concrete Bridge Columns Under Uncertainty

Author(s): *Christopher Eamon, Ahmad Alsendi, *Wayne State University*.

Bridge design in the United States is primarily governed by standards set by the American Association of State Highway and Transportation Officials (AASHTO) LRFD Bridge Design Specifications. These standards were calibrated to provide a minimum target reliability index to structural components of 3.5. Although the LRFD Specifications recognize the importance of blast loading, these standards do not contain corresponding design provisions in detail. Of particular importance are the bridge columns, which if severely damaged, may lead to the progressive collapse of the entire structure. Although analytical research has been conducted on modeling blast load effects on bridge columns and some guidelines for blast design have been proposed, the response of these critical bridge components under blast threats remains unclear, and the reliability of bridge columns under blast loads is largely unknown. Therefore, the development of a reasonably simple but accurate numerical model that can be used to predict the reliability of bridge columns under blast threats is needed, as well as a better understanding of the behavior of these structures and the effectiveness of protective measures. To address these issues, in this study, a large strain, large displacement numerical (finite element) model that allows element separation and failure is developed and validated based on existing results of blast experiments. In this model, concrete is represented with the Johnson-Holmquist-Cook model while a plastic-kinematic relationship describes steel behavior. This model is paired with a probabilistic Failure Sampling technique to account for uncertainties in blast load and material resistance parameters. The model is used to predict the response of typical bridge columns to blast loads, as well as to determine the reliability of bridge columns under these threats. Changes in design parameters such as concrete strength, steel reinforcement ratio, bridge live (vehicle) and dead load, and blast charge weight are considered in a probabilistic parametric analysis. Moreover, the effectiveness of a method of column protection is investigated, where existing columns are wrapped with a relatively inexpensive steel fiber reinforced polymer (SFRP) jacket. It was found that the use of SFRP can greatly minimize the effect of an explosive load on the columns, and represents a practical and effective method to increase column reliability level under blasts.

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14th U.S. National Congress on Computational Mechanics
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Title: Robust Polyhedral Meshing

Author(s): *Mohamed Ebeida, *Sandia National Laboratories*; Ahmed Abdelkader, *University of Maryland*; Ahmad Rushdi, *University of California Davis*.

In this talk, we introduce novel methods for Robust Polyhedral Meshing. These methods include innovative solutions to long-standing open problems in sampling, meshing, optimization, and uncertainty quantification and will be deployed in a new software package, called "VoroCrust". Our core algorithm aims to overcome major meshing design challenges including efficient handling of CAD models (e.g., automatic feature detection), adaptive sampling, unclipped Voronoi meshing of non-convex domains, and generating Voronoi cells without short edges. We utilize variations of maximal Poisson disk sampling for adaptive sphere packing covering the entire surface. Consequently, we carefully place seeds in the close vicinity of the surface to reconstruct it using the facets of unclipped Voronoi cells. We then fill the interior with well spaced seeds to produce cells with good aspect ratio everywhere. To our knowledge, this is the first robust tool to generate 3D Voronoi meshes that naturally conform to the input CAD model with no clipping. The output mesh is free of sliver artifacts and has a guaranteed quality (convex elements, planar facets, angle bounds, aspect ratio, etc). We also output an approximation of the medial axis and in-out point classification relative to the reconstructed surface. A variation of our algorithm generates weighted unclipped Voronoi cells in order to achieve more seed placement flexibility. We also include methods for mesh optimization via constrained resampling to achieve user desired quality objectives (e.g., generating Voronoi cells with no short edges). We finally demonstrate the innovative extension of our tools beyond classical meshing. For example: piecewise Surrogate Modeling, Calibration, Global optimization, automatic discontinuity detection and representation, and Linear programming.■

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14th U.S. National Congress on Computational Mechanics
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Title: Prediction from First Principles of the Structure and Composition of Vanadium Carbide Nanoprecipitates in Microalloy Steel

Author(s): *Sebastián Echeverri Restrepo, *SKF*; Davide Di Stefano, *Université catholique de Louvain*; Matous Mrovec, *Ruhr-Universität Bochum*; Michael W. Finnis, *Imperial College London*; Anthony T. Paxton, *King's College London*.

Currently there is great interest, and some controversy, surrounding the nature of the nano-sized vanadium carbides that are found in microalloy, bearing and other high strength steels. Recent experiments are able to reveal the size, the stoichiometry and the crystal structure of these precipitates; as well as identifying them as traps for hydrogen. What is not yet available is a scheme to predict the stoichiometry and crystal structure that can be expected to exist in equilibrium with austenite or ferrite having a given concentration of carbon and vanadium at a given temperature. We provide the beginnings of such a scheme by calculating mechanical and thermodynamic properties of five putative vanadium carbides, using first principles quantum mechanics. We provide evidence that cubic V4C3 phase that is commonly supposed to exist has an unfavourable heat of formation compared to competing crystal structures, while we demonstrate the correctness of our theory by applying it to a steel of known composition and heat treatment, whose carbides have been assessed in the electron microscope.

14th U.S. National Congress on Computational Mechanics
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Title: 2D Continuum Model for Simulating Angiogenesis Studies in Microfluidic Systems

Author(s): *Nikola Kuzmic Edmond W. K. Young, *University of Toronto*.

Tumor-induced angiogenesis is a process which involves growth of blood vessels from existing vasculature for purpose of increasing nutrient supply to undernourished parts of the tumor tissue. Being able to predict the growth and behavior of blood vessel networks under different stimuli is crucial to understanding the growth of tumors and ultimately designing better cancer treatment plans. Angiogenesis is an active area of research which has the potential to play a significant role in advancing cancer therapy [1]. It involves several cellular processes, including chemotaxis and haptotaxis. Chemotaxis refers to migration of endothelial cells (ECs) in response to vascular endothelial growth factor (VEGF) gradient and haptotaxis refers to migration of ECs along an adhesive chemical gradient, such as fibronectin (FN). While these angiogenesis processes have been modeled before, the models have yet to be applied to microfluidic systems, which are increasingly being used for experimental angiogenesis research. Performing experiments is costly and time consuming. Carrying out accurate simulations to investigate chemical influence on angiogenesis instead, would lessen the number of experiments required to draw conclusions. Our main goal is to study the effects of VEGF and FN (and other chemicals) on angiogenesis, specifically in a microfluidic context, in an accurate and efficient manner. In this paper, we present a 2D simulation of angiogenesis based on a continuum model proposed by Orme and Chaplain [2] inside the diffusion ports of our microfluidic device. The system is nondimensionalized and simulations are performed using FEniCS [3]. We apply constant FN concentration at four sections on the top side of the port and uniform constant concentration of ECs over the same side. Constant VEGF concentration is applied at the bottom of the port to represent realistic boundary conditions that would be found in a typical experimental setup. Results demonstrate both: chemotaxis and haptotaxis. The novelty of this study is integration of mathematical modeling with microfluidic devices to aid biologists and chemists in drug discovery. 1. Carmeliet, P. (2005). Angiogenesis in life, disease and medicine, Nature, Vol (438). 2. Orme, M. E., Chaplain, M. A. (1997), Two-dimensional models of tumor angiogenesis and anti-angiogenesis strategies, IMA Journal of Math. App. In Medicine & Biology, Vol (14), 189-205. 3. Alnaes, M. S., Blechta, J., Hake, J., Johansson, A., Kehlet, B., Logg, A., Richardson, C., Ring, J., Rognes, M.E., Wells, G. N., The FEniCS Project Version 1.5, Archive of Numerical Software, Vol (3).

14th U.S. National Congress on Computational Mechanics
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Title: Crack Detection by Scaled Boundary Finite Element Method and Global Optimization Algorithms

Author(s): *Adrian W. Egger, Eleni N. Chatzi, *ETH Zurich*; Savvas P. Triantafyllou, *University of Nottingham*.

Keywords: Scaled Boundary Finite Element Method (SBFEM), Crack Detection, Global Optimization Algorithms
Abstract: In this work, a novel crack detection scheme for structures is presented, which combines the scaled boundary finite element method (SBFEM) [1] with global optimization algorithms. Crack detection schemes [2] rely on adoption of optimization algorithms for solving the inverse problem of detection via minimizing the discrepancy between experimentally measured structural response and the estimated response, derived by means of numerical simulation. The design variables of these optimization procedures commonly comprise the parametrized crack geometry and location. The main computational effort in this invers procedure stems from the need to solve a considerable number of forward problems for different realizations of the crack geometry. SBFEM comprises a semi-analytical scheme, wherein an analytical solution in radial direction is obtained. This is accomplished by introducing a scaling center within the domain and therefore transitioning from a Cartesian reference system to one resembling polar coordinates. Consequently, the dimensionality of the computational domain is reduced by one, implying only discretization of the boundary in the finite element sense, which significantly accelerates the simulation procedure. Within the setting of fracture mechanics, SBFEM does not require the discretization of the crack, when the scaling center is placed at the crack tip, further reducing the computational toll. Additionally, via computation of the analytical limit as the stresses approach the crack tip, the stress intensity factors (SIFs) are extracted on the basis of their formal definition, without requiring any a priori knowledge and at negligible computational cost. In this work, emphasis is placed on the reduction of the computational cost associated with a single forward analysis with the overall aim of significantly increasing the computational speed of crack detection procedures. Furthermore, the performance of evolutionary algorithms such as the genetic algorithm (GA), the particle swarm optimization (PSO) and covariance matrix adaption evolution strategy (CMA-ES) [3] is assessed. Numerical examples demonstrate that the combination of SBFEM and global optimization algorithms significantly accelerates computation. References: [1] Wolf, J. (2003). The Scaled Boundary Finite Element Method (1st ed.). John Wiley & Sons. [2] Rabinovich, D., Givoli, D., & Vigdergauz, S. (2007). XFEM-based crack detection scheme using a genetic algorithm. International Journal For Numerical Methods In Engineering, 71(9), 1051-1080. [3] Hansen, N. & Ostermeier, A. (2001). Completely Derandomized Self-Adaptation in Evolution Strategies. Evolutionary Computation, 9(2), 159-195.

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Title: Modelling Hydraulic Fracturing as a Transition from Diffuse Micro-Cracking to Fracture Localization

Author(s): *Mahdad Eghbalian, *University of Calgary*; Richard Wan, *University of Calagry*.

The failure behavior of geomaterials is of widespread relevance in Geomechanics, including geo-environmental applications. A better understanding of the failure behaviour of such materials beyond traditional approaches is crucial in the design and performance of key infrastructures in civil/petroleum engineering problems. At issue, is the study of both mechanical and numerical aspects of fracture genesis and evolution in geomaterials. The current work aims at a more scientifically sound study of the fracture behaviour of saturated sedimentary rocks as a multi-physics/multi-scale process. The failure process of sedimentary rocks comprises an initial diffuse stage and an ultimate localized stage. In the current work, the material behaviour in the diffuse stage is described through a multi-scale model developed within a Homogenization framework. The proposed continuum model is thus embedded with microstructural information; specifically, the micro-cracks and their evolution are tracked at the continuum level through a directionally dependent variable (micro-crack distribution). To this end, a fracture criterion for micro-crack growth is introduced to capture the induced anisotropy at the macro-scale. The material eventually fails along a preferential direction through localization of micro-cracks to eventually give way to one or more macro-cracks. The current work addresses the transition from the gradual degradation of kinematics to the localized macro-crack emergence at the continuum level. The multi-scale model is incorporated in a numerical scheme based on eXtended Finite Element Method (XFEM) framework in view of a more reliable tool to simulate the discrete nature of the post-failure behaviour. The strong discontinuity in this method is modeled by enriching the displacement-based approximation near the macro-cracks. This is accomplished by incorporating both the discontinuous fields and near tip asymptotic fields in the approximation through the concept of reproducing kernels and the partition of unity method. As such, the mesh does not need to conform to the geometry of the macro-cracks and as a result, the numerical treatment can handle complex fracture patterns. This method is combined with the level-set method for tracing the crack propagation path and provides stable, mesh independent results. Numerical simulations of hydraulically-driven fractures are performed to show how the proposed model addresses the crack propagation problem more realistically, in the sense that the crack behaviour is a direct consequence of how the surrounding material behaves under the influence of microscopic cracks and cavities. We are especially interested in the overall enhancement achieved in the permeability of the medium under hydraulic loading.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: MESHFREE: General Finite Differences for Fluid Flow and Continuum Mechanics with Three Industrial Applications

Author(s): Joerg Kuhnert, *Almut Eisentraeger, Timo Waechtler, *Fraunhofer ITWM*.

The numerical tool MESHFREE is a further development of the so-called Finite Pointset Method (FPM), a purely grid-free approach to problems in continuum and fluid mechanics. The method is based on a general finite difference formulation in conjunction with an adapted least squares ansatz for higher order approximation properties. The fluid/continuum is represented by a moving cloud of numerical points. A generalized scheme covers the whole spectrum of problems of very small up to very large Reynolds (Re) and Strouhal (St) numbers. The numerical flow solver was developed in Fraunhofer ITWM. The big sparse linear systems evolving out of the implicit time integration are solved by the algebraic multigrid method (SAMG) by the Fraunhofer SCAI. In order to demonstrate MESHFREE's flexibility and the potentially high industrial applicability, we are going to show three different industrial cases: (1) Industrial sloshing, such as in tanks: Here, MESHFREE precisely predicts noise effects or heavy wave impact. Especially important is the interaction of the fluid with the air/gas contained in the tank. Therefore, we have developed the so called bubble algorithm, which avoids treating air as a second phase, but tracks bubbles as macroscopic entities representing closed partitions of the free surface with a unique internal pressure depending on the bubble’s compression; (2) Hydraulic return valve, used for example in conventional combustion engines: The simulation is used to model the opening and closing behaviour of the valve. If oil is pushed in one direction, the valve will open and oil starts to flow. If pushed in the other direction, a mechanism inside the valve closes and the oil flow is stopped. Basic questions here are the opening and closing times and the leakage flow. For this application, we have coupled MESHFREE with reduced FE-models for the flexible structures within the valve; (3) Water drain with wind: Two MESHFREE simulations are coupled with one another. One simulation models the wind around a vehicle structure, the other one models the water/spray flow of rain. The water flow is mostly governed by surface tension and contact angles. The focus here lies in the coupling procedure of both phases. Water drain is a subject of increasing importance to car industry. For all three applications, we show comparisons of the MESHFREE simulation results with experiments.

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Title: A New Hybrid Numerical Scheme For Simulating Fault Ruptures With Near Fault Bulk Inhomogeneities

Author(s): *Ahmed Elbanna, Setare Hajaroalsvadi, *UIUC*.

The Finite Difference (FD) and the Spectral Boundary Integral (SBI) methods have been used extensively to model spontaneously propagating shear cracks in a variety of engineering and geophysical applications. Although the SBI method is a computationally efficient and highly accurate scheme, its use is limited only to linear elastic homogeneous media with planar interfaces. The FD method, however, is more flexible and can handle material and geometric nonlinearities but is computationally demanding due to bulk discretization. We propose a new modeling approach, in which these two methods are combined through consistent exchange of boundary tractions and displacements. Benefiting from the flexibility of FD and the efficiency of spectral boundary integral (SBI) methods, the proposed hybrid scheme can solve a wide range of problems in a computationally efficient way. The main idea of the method is to enclose the inhomgeneities in a virtual strip that is introduced for computational purposes only. This strip is then discretized using a volume-based numerical method, chosen here to be the finite difference method while the virtual boundaries of the strip are handled using the SBI formulation that represents the two elastic half spaces outside the strip. Modeling the elastodynamic response in these two halfspaces needs to be carried out by an Independent Spectral Formulation before joining them to the strip with the appropriate boundary conditions. Dirichlet and Neumann boundary conditions are imposed on the strip and the two half-spaces, respectively, at each time step to propagate the solution forward. We illustrate the accuracy and efficiency of the method using several examples, the two prominent ones being a slip-weakening crack with a low-velocity fault zone and a slip-weakening crack with off-fault plasticity. This approach is more computationally efficient than pure FD and expands the range of applications of SBI beyond the current state of the art.

14th U.S. National Congress on Computational Mechanics
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Title: Multilevel-Multifidelity Expansions with Application to Emulator-Based Bayesian Inference

Author(s): *Michael Eldred, Gianluca Geraci, Alex Gorodetsky, John Jakeman, *Sandia National Laboratories*.

In the simulation of complex physics, multiple model forms of varying fidelity and resolution are commonly available. In computational fluid dynamics, for example, common model fidelities include potential flow, inviscid Euler, Reynolds-averaged Navier Stokes, and large eddy simulation, each potentially supporting a variety of spatio-temporal resolution/discretization settings. While we seek results that are consistent with the highest fidelity, the computational cost of directly applying UQ in high random dimensiona quickly becomes prohibitive. In this presentation, we focus on the development of multilevel-multifidelity surrogate models in order to fuse information from multiple fidelities and resolutions and reduce the overall computational burden. Within the general family of multivariate orthogonal polynomial expansions, we will focus on the development of approaches that are appropriate for large-scale emulation through the exploitation of sparse and low rank structure, including compressed sensing and tensor train approaches. These multilevel-multifidelity emulators will be deployed to the Markov-chain Monte Carlo sampling process using accelerations based on emulator gradients and Hessians, and demonstrated for both model problems and engineered systems such as high-performance aircraft nozzles.

14th U.S. National Congress on Computational Mechanics
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Title: Simulating Drug-Affected Cardiac Electromechanics

Author(s): *Khalil Elkhodary, Noha Shalaby, *American University-Cairo*; Nejib Zemzemi, *Carmen Group*.

In this work an imaged physiological model of the human ventricles is studied by the finite element method, on the multiscale/multiphysics solver Chaste. We focus on improving the description of the passive component of the force, including its dependence on the alignment of myofibers, to better investigate the effect of drugs on cardiac electro-mechanics. We rely on an established model from Chaste for the active component. To model the flux of ions and associated electrical activity of an individual myocyte in humans under the inhibitory effect of a specific drug dosage on the ionic channels, a modification is imparted to the Ten Tusscher and Panfilov action potential model. The current calculated by the ionic model is then fed back to the monodomain equation. A Na+ channel blocker and a K+ channel blocker were separately applied and their electromechanical results studied. Our predictions indicated that a delay in the electrical activation of ventricular tissue caused by a Na+ channel blocker translates to a delay in all the mechanical biomarkers we investigated for the ventricles, consistent with the literature. However new predictions were also made; Na+ channel block increases left ventricular twist and increases radial stretching/shortening at the base of the ventricles by measurable amounts. For K+ channel block our electrophysiological predictions showed no alteration to tissue activation time, but only a prolonged QT interval, consistent with literature. Limited by our choice of the Kerchhoff active stress model on Chaste, the mechanical predictions were the same as for the control.

14th U.S. National Congress on Computational Mechanics
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Title: Aerodynamic Mitigation of Tall Buildings Using Local and Global Shape Optimization

Author(s): *Ahmed Elshaer, Girma Bitsuamlak, *Western University*.

Wind design is a governing load case for tall buildings. The dependency of wind load on the outer shape of a tall building provides a unique opportunity to reduce the wind-induced forces and vibrations. Many numerical and experimental studies are reported that investigated the efficiency of different mitigations types (i.e. local and global mitigations) to improve the aerodynamic performance of tall buildings. However, comparing limited building alternatives can only produce an ad-hoc solutions rather than optimal solutions. In this study, an optimization technique is integrated with aerodynamic assessment method that results in wider search space thus producing more aerodynamic shapes, which results in optimal reductions in the wind load and consequently the overall cost. For this purpose, an aerodynamic optimization procedure (AOP) is developed, which couples Genetic Algorithm, Computational Fluid Dynamics (CFD) and an Artificial Neural Network surrogate model in an automated process. This procedure is then adopted to optimize tall buildings both using local (corner modification) or global (twisting, through opening) mitigations, by conducting CFD simulations of three-dimensional turbulent wind flow for various wind directions. The procedure is examined in multi-objective optimization problems by defining the Pareto-Front, which allow architects and engineers to select optimally performing geometric parameters with respect to strength and serviceability considerations.

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Title: Stress-Constrained Level Set Topology Optimization for Compliant Mechanisms

Author(s): *Hélio Emmendoerfer Junior, Emílio Carlos Nelli Silva, *University of São Paulo*; Eduardo Alberto Fancello, *Federal University of Santa Catarina* .

This work presents a level set framework to solve topology optimization problems of compliant mechanisms subject to local stress constraints. Two technical difficulties are related to this problem. The first one is the local nature of stresses. To deal with this issue, stress constraints are included to the problem by means of an augmented Lagrangian scheme. The second are the unwanted flexible joints (hinges) usually obtained in flexible structure designs. This difficulty is overcome by controlling the von Mises stresses level. In the present approach, a reaction-diffusion equation substitutes the classical Hamilton-Jacobi equation to control the level set evolution. This choice has the advantage of allowing the nucleation of holes inside the domain and the elimination of the undesirable level set reinitializations. In order to validate the proposed scheme, benchmark numerical examples are presented in addition to an application for designing a pressure actuated compliant mechanism. Keywords: Topology optimization; Level Sets; Local stress constraints; Compliant mechanisms

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Title: Mesh Quality of Mixed-Element Bernstein-Bezier Meshes

Author(s): *Luke Engvall, John Evans, *University of Colorado Boulder*.

Higher-order mesh generation has enjoyed increasing popularity in recent years, as it promises to provide both improved geometric fidelity and more accurate simulation results when compared to traditional linear mesh generation. Recently, we have developed a framework for creating higher-order mixed-element meshes composed of Bernstein-Bezier tetrahedra, hexahedra, wedges and pyramids that are both geometrically exact and analysis suitable. Generally speaking, our framework requires only two things 1) a suitable underlying linear mesh and 2) a suitable CAD file of the surface. As a result, the framework is easily used alongside existing mesh generation technologies to create geometrically exact meshes of complicated objects, which we have demonstrated in our recent work. Furthermore, we have also demonstrated by example that the resulting meshes are analysis suitable. However, an outstanding challenge has been that of enforcing a-priori user defined constraints on mesh quality. In this talk we will focus on three key aspects of our recent work. First, we will provide a short overview of our meshing framework. Second, we will elaborate on some of the challenges related to mesh quality in our framework. Specifically, we have established sufficient mesh quality conditions that guarantee optimal convergence rates for higher-order Bernstein-Bezier meshes, and we will discuss several strategies for generating meshes that satisfy these conditions. Finally, we will discuss the effect of mesh quality on the analysis suitability of these meshes.

14th U.S. National Congress on Computational Mechanics
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Title: Predicting Lung Motion with Autodesk Simulation

Author(s): *Jaesung Eom, *Autodesk*.

This talk presents predicting lung motion with computational mechanics application from Autodesk. Respiratory motion has a profound impact on radiation therapy and diagnostic imaging of the lungs due to unique spatially and temporally variant tissue properties. Although the general biomedical studies of the lungs have a relatively long history, dynamic modeling of lung motion is relatively new, enabled by recent advances in computational and imaging technologies. We propose an inverse finite element-based technique to compute subject-specific parameters of soft tissue material models from patient-specific 4D CT images. The procedure is clinically relevant as the parameter identification involves minimization of an objective function which is defined by measuring the error between the observed and predicted displacements at multiple landmark points, chosen by expert radiologists, over multiple breathing phases.

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Title: Simulating Interfacial Multi-Physics Problems Using a Meshfree Approach

Author(s): *Lindsay Erickson, Jeremy Templeton, Karla Morris, *Sandia National Laboratories*.

Modeling the thermal-mechanical properties of molten metal for applications such as additive manufacturing proves challenging for finite element methods when geometry changes and liquid relocation occur. In addition, correctly capturing the surface curvature and residual stress are crucial to these thermal-mechanical applications. Particle methods such as smooth particle hydrodynamics (SPH) have been applied to molten metal, since these types of methods are better suited for moving boundary problems but the SPH formulation precludes verification. Alternatively, the Reproducing Kernel Particle Method is amenable to rigorous error analysis by retaining the integral form. Given this promise, we have developed a mesh-free method capable of resolving solid-to-liquid interfacial physics. We propose a new particle level set method to track the melting front and air-liquid interface combined with the Reproducing Kernel Particle Method for the background fluid and solid heat calculations and finite element methods for the residual stress calculations. Tracking a melt front is complicated by the fact that the interfacial velocity must be distinguished from the flow velocity. The mass flux between phases at the interface will be equal to the jump in heat flux across the interface over the latent heat of phase change. Using the Stefan condition, the interfacial velocity is solved for in terms of the mass flux and fluid velocity. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
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Title: Numerical Model of Fracture Initiation from Perforated Wellbore

Author(s): *Denis Esipov, Dmitriy Kuranakov, Vasiliy Lapin, Sergey Cherny, *Institute of Computational Technologies SB RAS*.

There are cases in the practice of hydraulic fracturing when the fracture does not start. The wellbore pressure increases significantly, but the breakdown conditions are not fulfilled. In addition, oil engineers want to make fracture in the desired direction. So that, it is necessary to investigate the process of fracture initiation. It is a challenging task due to the complex geometry of the perforated wellbore and heterogeneity of the real rock medium. The first reason forces us to consider fully 3D problem statements without any simplifications, while the second one necessitates the usage of special breakdown criteria. This report presents a numerical model of fracture initiation, which consists of three main parts. The first one is a computation of stress-strained state of a rock around perforated wellbore by the boundary element method in accordance to linear elasticity theory. The second is a computation of the breakdown pressure by applying the breakdown criterion for every point on the wellbore and perforation surfaces. The last is the construction of the surface of incipient fracture wedged into the rock. The main advantage of our model is the usage of the wide range of criteria, from simple maximum tensile stress criterion to advanced criterion accounting the size effect. One of them is our developed R-criterion, which takes into account the size effect without using information on sizes of specimen. Therefore, it is convenient for practical applications for problems with complex geometry. We have performed computations for various geometries of perforated wellbore and found typical fracturing scenarios. Besides the usual scenario when the fracture starts from the tip of one perforation, there are many situations when the fracture starts from the wellbore side or the wellbore-perforation junction. The in-situ stresses, wellbore orientation, geometry and direction of perforations and the type of the rock have the main influence on the scenario of fracture initiation as well as on the magnitude of the breakdown pressure. Several comparisons of the computed results with the laboratory experiments will be demonstrated.

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14th U.S. National Congress on Computational Mechanics
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Title: Characterization of Airway Wall Mechanics

Author(s): *Mona Eskandari, Alberto Arvayo, Marc Levenston, Ellen Kuhl, *Stanford University*.

Lung disease is the third leading cause of death in the United States and has an even higher fatality rate in countries with excessive pollution. Strikingly, pulmonary mechanics and airway obstruction remain drastically understudied. To date only a handful of studies have explored the material properties of the airway walls, and most have been restricted to the trachea, the largest, most accessible passageway [1, 2, 3]. Computational models have been limited by the availability of airway material properties, utilizing the trachea to infer the mechanics of diseases affecting the small bronchi and bronchioles [4]. Furthermore, the pertinent viscoelasticity of the airways has been overlooked [5]. Here we address the pressing need for airway-specific material characterization to inform the biophysical response of the airway tree. To characterize orientation- and region-dependent tissue response, fresh lungs from five pigs (>6 months) were used to prepare six sets of test specimens (~30 samples/set) from three regions (trachea, large bronchi, and small bronchi) and two directions (axial and circumferential). Displacement controlled uniaxial tensile tests revealed the stress-strain and viscoelastic response. Substantial heterogeneity and anisotropy of the airway tree was found ($p<0.05$ or less). The stiffness modulus, defined as the slope of the linear portion of the stress-strain curve, was significantly larger axially than circumferentially (33kPa vs. 9kPa); the small bronchi stiffer circumferentially than the trachea and large bronchi (13.5kPa vs. 6.8kPa). As for stress relaxation, defined as the ratio of peak stress to diminished stress after 300s, circumferential samples exhibited greater stress relaxation than axial counterparts (0.38 vs. 0.22), and both axial and circumferential trachea samples displayed greater stress relaxation (0.26 and 0.43) than large bronchi and small bronchi counterparts. To the best of our knowledge, this is the first documentation of the mechanical properties of small bronchi, the predominant site of disease. These experiments equip us with airway-specific constitutive relations and demonstrate the anisotropic and heterogeneous nature of proximal to distal airways. Furthermore, the results facilitate clinical deductions regarding ventilated induced lung injury (VILI) and parenchymal mechanics, and directly enable computational tools for predicting obstruction in chronic lung disease. References: [1] Codd, SL et al., J Appl Physiol, 76.6: 2627-2635, 1994. [2] Noble, P et al., J Appl Physiol, 99.6: 2061-2066, 2005. [3] Teng, Z et al., J Biomech, 45.9: 1717-1723, 2012. [4] Eskandari, M et al., J Theor Biol, 403: 209-218, 2016. [5] Fung, Y, Biomechanics: Mechanical Properties of Living Tissues, 2013.

14th U.S. National Congress on Computational Mechanics
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Title: A Critical Comparison of Coupling Schemes for Non-Matching Isogeometric/Finite Element Discretizations

Author(s): *John Evans, Eric Peters, *University of Colorado Boulder*.

Despite the growing popularity of isogeometric analysis, a large majority of analysis codes are built on finite element or related discretizations. Thus, an important step toward wide-spread adoption of isogeometric analysis is to mate isogeometric analysis with classical finite element analysis. Moreover, to bridge this gap, there is a great need for stable, efficient, and accurate coupling schemes for non-matching isogeometric/finite element discretizations. In this talk, we provide a critical comparison of such schemes, with a focus on the following six characteristics: (i) stability, (ii) accuracy, (iii) locality, (iv) kinematic (or primal field) conservation, (v) kinetic (or flux field) conservation, and (vi) ease of implementation (both in staggered and monolithic solution environments). To set the stage, we first provide a unified variational framework for (parametrically and geometrically) non-matching interface treatment. Our framework encompasses many popular interface treatments, including the methods of Lagrange multipliers, dual Lagrange multipliers, and stabilized Lagrange multipliers. We then present stability and convergence criteria for the unified framework in the context of a simplified model problem, as well as necessary criteria for kinematic and kinetic conservation. Using these criteria, we compare and contrast several common coupling schemes for non-matching discretizations as well as a selection of new, non-standard approaches. We then discuss challenges faced by each of these approaches in terms of computational cost and intrusiveness of implementation. We conclude by examining the accuracy and stability of these coupling schemes as applied to acoustic-structure and fluid-structure interaction by numerical example.

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Title: Discontinuous Galerkin Approximation of Flows in Fractured Porous Media on Polytopic Grids

Author(s): Paola Francesca Antonietti, *Chiara Facciolà, *Politecnico di Milano, Dipartimento di Matematica, MOX-Laboratory for Modeling and Scientific Computing*; Alessandro Russo, *Università degli Studi di Milano-Bicocca, Dipartimento di Matematica e Applicazioni, & IMATI-CNR Pavia*; Marco Verani, *Politecnico di Milano, Dipartimento di Matematica, MOX-Laboratory MOX-Laboratory for Modeling and Scientific Computing*.

We present a numerical approximation of Darcy's flow through a fractured porous medium which employs discontinuous Galerkin methods on polytopic grids. We adopt the model for single-phase flows proposed in [1], that is valid for fractures with both large and low permeability. This model considers the case of a single fracture, treated as a (d -1)-dimensional interface between two d-dimensional subdomains, d = 2, 3. The flow in the porous medium is assumed to be governed by Darcy's law and a suitable reduced version of this law is formulated on the surface modelling the fracture. Physically consistent coupling conditions are added to account for the exchange of fluid between the fracture and the porous medium. We focus on the numerical approximation of the coupled bulk-fracture problem, employing Discontinuous Galerkin (DG) finite elements on polytopic grids. The choice of DG methods arises spontaneously in view of the discontinuous nature of the solution at the matrix-fracture interface. However, this is not the only motivation. Indeed, the interface conditions can be naturally formulated using jump and average operators and embedded in our variational formulation, so that DG methods turn out to be a very powerful approach for handling the (weak) coupling of the two problems. The DG method that we propose can handle arbitrarily-shaped polytopic grids, made of elements with edges/faces that may be in arbitrary number and whose measure may be arbitrarily small [2,3]. The use of computational meshes made of general polytopic elements is naturally well suited to handle complicated geometries and is made in view of extending the formulation to the case of networks of fractures. We theoretically analyze our discrete formulation, prove its well-posedness and derive optimal a priori error estimates in a suitable (mesh-dependent) energy norm. Finally, we present numerical experiments assessing the validity of the theoretical error estimates. [1] V. Martin, J. Jaffré, J.E. Roberts. Modeling fractures and barriers as interfaces for flow in porous media. SIAM J. Sci. Comput. 26:1667-1691, 2005. [2] A. Cangiani, Z. Dong, E.H. Georgoulis. hp-Version space-time discontinuous Galerkin methods for parabolic problems on prismatic meshes. arXiv preprint:1605.01212, 2016. [3] P.F. Antonietti, A. Cangiani, J. Collis, Z. Dong, E.H. Georgoulis, S. Giani, P. Houston. Review of discontinuous Galerkin finite element methods for partial differential equations on complicated domains. Lecture Notes in Computational Science and Engineering, 2016.

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Title: The Materials Science of Chemically Driven Elastic Incompatibility: A Multi-Physics Study of Lithium Ion Battery Electrode Li_(1+x) Ti_2 O_4

Author(s): *Michael Falk, Tonghu Jiang, *Johns Hopkins University*; Shiva Rudraraju, Krishna Garikipati, *University of Michigan*; Anton Van der Ven, *University of California, Santa Barbara*.

Recently, a huge materials space is being explored for cheaper, higher energy density, and reliable battery materials, due to the growing demand of portable electronics and electric vehicles. During charge and discharge cathodes of lithium ion batteries typically undergo first order phase transformations. The resulting two-phase coexistence can lead to elastic incompatibilities that drive failure and limit lifetime. In this work, we use a series of computational tools to study the thermodynamics and kinetics of Li1+xTi2O4. Density functional theory (DFT) calculation was used to obtain formation energies with different lithium configurations, and migration barriers for lithium ion transitions. The cluster expansion method is employed to approximate these energies. These are then deployed to develop physics-based parameterizations of the relevant structural and kinetic properties that inform a phase field model in order to simulate this material at macroscopic level. The development of internal stresses during charging and discharging is simulated and analyzed with an eye to understanding how these lead to electrode degradation and failure.

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Title: Potential Energy Landscape and Dynamics of Inherent Structure Evolution in Metallic Glasses

Author(s): *Yue Fan, *University of Michigan*.

The studies on dynamics in glassy materials are particularly challenging because of their strongly disordered atomic nature. In the picture of potential energy landscape (PEL), the evolution of inherent structure (IS) energy can be attributed to the competitions between activations and relaxations. In particular, whether glasses will undergo aging or rejuvenation depends on whether the activation barrier is smaller or larger than the relaxation energy. We prepared 6 metallic glass samples with different thermal histories (from 1013K/s to 109 K/s), and further explored their activation barrier and relaxation energy spectra through advanced atomistic sampling technique. The spectra are found sensitive to the systems' IS energy. Stemmed from such dependence, a self-consistent equation in describing IS energy evolution has been derived. Without any empirical parameter, this equation can well explain the equilibrium line of supercooled liquid and the cooling curves at different rates directly obtained by MD studies.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Crashworthiness Optimization of Horsetail-Bionic Thin-Walled Structures

Author(s): *Hongbin Fang, *Univ. North Carolina-Charlotte*; Youye Xiao, Hanfeng Yin, Guilin Wen, *Hunan University*.

Bio-inspired engineering design has drawn increased attention in recent years for the excellent structural and mechanical properties of the biological systems. In this study, the horsetail-bionic thin-walled structures (HBTSs) were investigated for their crashworthiness under axial dynamic loading. Six HBTSs with different cross section configurations (i.e., number of cells) were evaluated using nonlinear finite element (FE) simulations. To obtain the optimal design of the HBTSs, an ensemble metamodel-based multi-objective optimization method was employed to maximize the specific energy absorption while minimizing maximum impact force of the HBTSs. Using ensemble metamodeling combined with FE simulations and the NSGA-II algorithm, the Pareto optimum designs of all six HBTSs were obtained and the HBTS with 16 cells were found to have the best overall crashworthiness. An optimum design of the HBTS with 16 cells was verified using FE simulation and found to have good agreement with simulation results.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Parametric Nonlinear Model Order Reduction Framework for Steady-State Flows Past Parametrically Deformed Complex Geometries

Author(s): *Charbel Farhat, *Stanford*; Kyle Washabaugh, *Boeing Commercial Aircraft*.

A parametric, nonlinear, Computational Fluid Dynamics (CFD)- and Projection-based, Model Order Reduction (PMOR) framework for the real-time solution of steady-state flow problems arising in aerodynamic shape what-if scenarios is presented. It features an optimal Petrov-Galerkin projection method [1] that preserves numerical stability, a hyperreduction approach designed around the concept of a reduced CFD mesh, and a mesh deformation scheme borrowed from computer graphics techniques that can operate on disjoint reduced CFD meshes. Using this computational framework, a nonlinear, CFD- and Projection-based Reduced-Order Model (PROM) is built with solution snapshots that are pre-computed offline for deformed geometries sampled by a feasible greedy procedure, clustered, and finally compressed into a series of local Reduced-Order Bases (ROBs) [2]. When a steady-state aerodynamic response is sought online for an unsampled geometry, an appropriate initial solution is first computed by interpolating the training data. Next, this initial solution is improved using a parametric PROM and a Newton-like procedure designed to minimize the norm of a scaled residual for the geometry of interest. The speed and robustness of the proposed computational framework for parametric nonlinear PMOR are demonstrated for two case studies: one focused on NASA's Common Research Model (CRM), which is representative of the aerodynamics of modern airline jets such as the Boeing 767, and one centered on the 2009 Volkswagen Passat. Accurate solutions of aerodynamic shape what-if problems are computed in both cases in real-time. [1] K. Carlberg, C. Farhat, J. Cortial and D. Amsallem, The GNAT Method for Nonlinear Model Reduction: Effective Implementation and Application to Computational Fluid Dynamics and Turbulent Flows, Journal of Computational Physics, Vol. 242, pp. 623-647 (2013) [2] D. Amsallem, M. Zahr and C. Farhat, Nonlinear Model Order Reduction Based on Local Reduced-Order Bases, International Journal for Numerical Methods in Engineering, Vol. 92, pp. 891-916 (2012)

14th U.S. National Congress on Computational Mechanics
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14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Model Discrepancy Calibration Across Experiments

Author(s): *Kathryn Farrell-Maupin, Laura Swiler, *Sandia National Laboratories*.

Despite the continuing advances in statistical inversion and modeling, model inadequacy due to model form error remains a concern in all areas of mathematical modeling, including computational mechanics. Introducing a model discrepancy formulation into the Bayesian framework can improve the predictive power of a given model and, arguably, the transferability of physical parameters. However, much like physical models, calibrating a discrepancy model requires careful consideration regarding formulation, parameter estimation, and uncertainty quantification, which is often problem-specific. We demonstrate a generalized approach and implementation of model discrepancy detection, construction, and propagation into a predictive setting, and provide an application to computational mechanics.

14th U.S. National Congress on Computational Mechanics
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Title: Quantifying the Volumetric Growth in an In Vivo Murine Glioma Using a Linear Mechanically-Coupled Model

Author(s): *Xinzeng Feng, David Hormuth, Thomas Yankeelov, *University of Texas at Austin*.

Introduction: There is an established body of experimental literature indicating the important role of solid stress in the process of glioma growth [1]. These studies motivate the incorporation of solid stress in tumor growth modeling. On the other hand, it is well known that in vivo tumor growth is highly non-uniform due to, for example, heterogeneity in cancer cells, extracellular matrix properties, level of solid stress and nutrient concentration. However, there are limited attempts to quantify such non-uniform growth in vivo. In this project, we propose to apply a linear mechanically-coupled model to quantify the non-uniform volumetric growth in an in vivo rat glioma based on magnetic resonance imaging (MRI) data. Methods: Diffusion-weighted MRI data were collected on female Wistar rats with C6 tumors at seven time points over two weeks. After image registration, the imaging data were converted to the estimated cellularity in each tumor voxel [2]. By comparing the distribution of cellularity at two time points, we estimate the spatiotemporal development of the tumor. More specifically, the tumor is treated as a growing elastic solid confined by the surrounding brain tissues, and growth is quantified by a scalar field representing local volumetric expansion. Using a state-of-art inverse-method algorithm, the distribution of local volumetric expansion is optimized iteratively so as to minimize the difference between the predicted cellularity and the measured cellularity at the second-time point. Results: Preliminary results on 2D image slices has demonstrated the capability of our approach to identify regions in the tumor with high volumetric growth. Summary of Presentation: We will present an efficient numerical approach to quantify the non-uniform volumetric growth of a rat glioma tumor based on in vivo MRI data. This technique will facilitate predictive modeling of in vivo glioma growth with quantitative estimation of the spatiotemporal growth and stress distribution. Results on multiple sets of real data will be presented. References: [1] Triantafyllos Stylianopoulos et al. “Causes, consequences, and remedies for growth-induced solid stress in murine and human tumors”. In: Proceedings of the National Academy of Sciences 109.38 (2012), pp. 15101–15108. [2] David A Hormuth II et al. “Predicting in vivo glioma growth with the reaction diffusion equation constrained by quantitative magnetic resonance imaging data”. In: Physical biology 12.4 (2015), p. 046006. Acknowledgments: We thank the NCI for funding through R01 CA138599, R21 CA169387, U01 CA174706, R25 CA092043, P30 CA68485, and from CPRIT RR160005.

14th U.S. National Congress on Computational Mechanics
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Title: A Fully Coupled Space-Time Multiscale Modeling Framework for Predicting Tumor Growth

Author(s): *Yusheng Feng, Mohammad Rahman, *UT San Antonio*; Tom Yankeelov, *UT Astin*; J. Tinsley Oden, *UT Austin*.

In this talk, a fully coupled space-time multiscale framework for modeling tumor growth is developed. The framework consists of a tissue scale model, a model of cellular activities, and a subcellular transduction signaling pathway model. The tissue, cellular, and subcellular models in this framework are solved using partial di erential equations for tissue growth, agent-based model for cellular events, and ordinary di erential equations for signaling transduction pathway as a network at subcellular scale. The model is calibrated using experimental observations. The results show that the model is capable of predicting major characteristics of tumor growth such as the morphological instability, growth patterns of di erent cell phenotypes, compact regions of the higher cell density at the tumor region, and the reduction of growth rate due to drug delivery.

14th U.S. National Congress on Computational Mechanics
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Title: Experience and Challenges with Part-Scale Modeling of Select Laser Melting Additive Manufacturing

Author(s): *Robert Ferencz, *Lawrence Livermore National L*; Neil Hodge, Rishi Ganeriwala, Ryan Vignes, *Lawrence Livermore National Laboratory*.

Many researchers are exploring thermomechanical modeling of the selective laser melting (SLM) process to gain insights into residual stresses and distortions arising during this additive manufacturing process. This is a challenging problem due to the range of scales: temporally from miliseconds for local material transformation to hours and days for overall part fabrication; spatially from 100 microns for the local melt pool versus overall part dimensions. Various approaches are being pursued to identify and implement abstractions rendering the problem computationally tractable while still yielding results providing meaningful insights. We are adapting a general purpose, nonlinear thermal-mechanical finite element code to model the SLM process. First touching upon some of our earlier successes modeling SLM for a stainless steel [1], we then survey challenges we have encountered as we attempt to model more general configurations and material systems. These difficulties have motivated reexamination of our assumptions and approaches, pointing the way toward more general and robust modeling. References [1] N.E. Hodge, R.M. Ferencz and R.M. Vignes, “Experimental comparison of residual stresses for a thermomechanical model for the simulation of selective laser melting”, Additive Manufacturing, 12, 169-168 (2016). [2] W.E. King, A.T. Anderson, R.M. Ferencz, N.E. Hodge, C. Kamath, S.A. Khairallah, “Overview of modeling and simulation of metal powder bed fusion process at Lawrence Livermore National Laboratory”, Material Science & Technology, 31, 957-968 (2015).

_____ This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-725626

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Sequential Estimation of Tissue Properties and Boundary Condition Parameters for Large Artery Hemodynamics

Author(s): *C. Alberto Figueroa, *University of Michigan*.

A major challenge in constructing three-dimensional patient-specific hemodynamic models is the calibration of boundary condition and material parameters that enable model predictions to match patient data on flow, pressure, wall motion, etc. acquired in the clinic. We have implemented a parameter estimation framework based on reduced-order Kalman filtering [1, 2] to estimate the Windkessel parameters that characterize the outflow boundary conditions in a 3-D subject-specific fluid-structure interaction model of aortic hemodynamics. We first demonstrate the suitability of this methodology to recover estimates and covariance metrics of tissue stiffness in an idealized model using synthetic data. Then, we estimate outflow boundary condition parameters in a clinical scenario: The estimation algorithm incorporates noninvasive flow data acquired using magnetic resonance imaging and pressure data from applanation tonometry in a healthy human volunteer and successfully produced converged estimates for the subject-specific aorta model. Numerical experimentation suggests that having time-resolved flow measurements in the branches of the model and pressure data at a single location is sufficient for the successful recovery of the boundary condition parameters. References [1] SJ Julier et al. P Amer Contr Conf 3(3):1628-1632 (1995). [2] P Moireau et al. Biomech Model Mechanobiol 11(1):1-18 (2012).

14th U.S. National Congress on Computational Mechanics
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Title: A Formulation for Cardiopulmonary Circulation Hemodynamics: Bridging Analytical Morphometry-Based Arterial Tree Models and Image-Based 3D Models Using Impedance Boundary Conditions

Author(s): *Vasilina Filonova, C. Alberto Figueroa, *University of Michigan*.

Idiopathic pulmonary arterial hypertension is a treatable but still incurable disease. Progressive thickening and/or stiffening of distal pulmonary vessels yield to an increase in pulmonary arterial pressure which can lead to fatal right heart failure. Multi-resolution and multi-scale modeling can be used to study the complexity of the underlying disease mechanisms. Key components that must be incorporated in the modeling effort include: a morphometry-based model of blood flow in the distal pulmonary arterial tree; a high-resolution, image-based 3D hemodynamic model; appropriate characterization of the model parameters; and, most importantly, growth and remodeling formulations to describe the disease progression in proximal and distal vessels. The present work is the first and fundamental step, which focuses on developing a hemodynamic model of the cardiopulmonary circulation. This model will enable defining homeostatic baseline states for the subsequent growth and remodeling studies. The novelty of our proposed cardiopulmonary circulation model lays in combining a computational 3D model of proximal vessels with analytical 2D models of distal arterial tree. Pulsatile blood flow is considered using fluid-structure simulations. The 3D component is image-based and patient-specific. Methodologically, we utilize a coupled-momentum method [1] for modeling the fluid-solid interactions, and a coupled multidomain approach for defining outflow impedance boundary conditions utilizing a Dirichlet-to-Neumann framework. The impedance boundary condition is calculated from analytical solutions utilizing Womersley's 2D theory of pulsatile flow in tethered deformable vessels [2]. Calculation of the impedance requires knowledge of the morphometry of the human pulmonary tree [3]. Here, we use available open-literature data based on the diameter-defined Strahler ordering system. References: [1] C.A.Figueroa et al., Comput. Methods Appl. Mech. Engrg., 195 (2006), 5685-5706. [2] M.S.Olufsen et al., Ann. Biomed. Eng., 28 (2000), 1281-1299. [3] R.L.Spilker et al., Ann. Biomed. Eng., 35 (2007), 546-559.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Towards a Multi-Fidelity Hemodynamic Model Pipeline for the Analysis of Cardiovascular Flow Under Uncertainty

Author(s): *Casey Fleeter, *Stanford Univ., Sandia Natl Lab*; Daniele Schiavazzi, *University of Notre Dame*; Alison Marsden, *Stanford University*; Gianluca Geraci, *Sandia National Lab*; Andy Kahn, *UCSD*.

Hemodynamic models are increasingly being successfully employed in the diagnosis and treatment of cardiovascular disease and surgical planning. However, their widespread adoption is hindered by their inability to account for uncertainty stemming from multiple sources. Under these conditions, a deterministic description of the hemodynamic response provides limited information of the process under study. This motivates the transition to a stochastic framework where modeling parameters are defined in probability with distributions either assumed or assimilated from available patient-specific data. A possible approach to performing stochastic analysis on these systems, while maintaining reasonable computational cost, is to leverage multiple varying-fidelity models of the same cardiovascular flow. Hemodynamic modeling generally consists of anatomic model construction from medical image data, followed by solution of the incompressible Navier-Stokes equations governing blood flow in elastically deformable vessels. However, further simplifying assumptions can be made to generate models of “intermediate complexity.” Details of the one-dimensional formulation, along with the numerical solution method used in this study, are given in [1]. We propose an automatic pipeline in which the one-dimensional model is generated based on the vessel centerline paths and segmentations created in the SimVascular open-source software suite [2] from patient-specific medical images. The results of our validation study, comparing the flow and pressure waveforms obtained from the one-dimensional and three-dimensional solvers, confirm the consistency of the model outputs with various input waveforms and boundary conditions. The results are also consistent with the formulation differences of the two underlying solvers. The wall material model of the one-dimensional solver versus the rigid wall formulation considered in SimVascular justified the observed difference in outputs. Finally, various approaches for non-intrusive uncertainty propagation were first validated on simple one-dimensional parametric models and differential Windkessel circuits, and successively used to characterize output uncertainty in one-dimensional hemodynamics. References: [1] Wan, J et al., Comput Method Biomec, 5:195–206, 2002. [2] Updegrove, A et al., Ann Biomedical Engg, 44:1–17, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: Numerical Implementation Aspects of a Constitutive Model for Concrete with a Deviatoric Shape of Yielding Surfaces Based on Bézier Curves

Author(s): *Paula Folino, *Universidad de Buenos Aires, F.*

The aim of this work is to present some details related to the numerical implementation of a highly non- linear 3D constitutive formulation for concrete so called the Performance Dependent Model [Folino & Etse 2012] in a finite element code. One of the relevant features of the model is it C-1 continuous yielding surface. While the meridians are described by second order polynomials, the deviatoric views were originally described by the well-known elliptical interpolation between the compressive and tensile meridians proposed by Willam & Warnke (1974). Afterwards, an alternative geometrical description of the deviatoric shape was explored, using Bézier polynomials. Although three different options were evaluated, involving quadratic, cubic and rational quadratic Bezier curves, only the two latter were found suitable for representing a real alternative to the elliptical interpolation approach. The numerical implementation of complex constitutive models taking into account the incidence of the third invariant, still nowadays, can be considered a challenge. It is usual to find in the literature that this incidence is neglected and circular deviatoric shapes are considered even for concrete like materials, particularly when non local formulations are considered or multiscale approaches are used. In this case, for the stress integration of the model, the backward Euler method was applied. A direct method was used that leads to a single iteration process, while full consistency condition was used for the determination of the plastic multiplier. The consistent tangent operator was obtained and used in the numerical approach. At the finite elements level, the arc length method combined with Newton's method was applied. In this work, some details of this implementation are presented, with focus on the comparison of different numerical aspects when Bézier curves are considered versus the elliptical interpolation approach. References [1] Folino, P., Etse, G., 2012. Performance dependent model for normal and high strength concretes. International Journal of Solids and Structures, 49 (5), 701–719. [2] K. Willam and E. Warnke, 1974, "Constitutive model for the triaxial behavior of concrete", Proc. Intl. Assoc. Bridge Struct. Engrg., Report 19, Section III, Zurich: 1-30. [3] Folino, P., Smilovich, D., 2015. Proposal of an interpolation function between the compressive and tensile meridians of failure and yielding concrete surfaces based on Bezier curves", 1st Pan-American Congress on Computational Mechanics, ISBN 978-84-943928-2-5, International Center for Numerical Methods in Engineering (CIMNE), pp.261-271.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Finite Deformation Constitutive Models and Mechanics of Peridynamic Mixtures

Author(s): *John Foster, Xiao Xu, *UT-Austin*.

The conservation of momentum equations for superimposed interacting materials, i.e. mixtures, can be rigorously derived using an extension of Hamilton's principle whereby constraint equations are appended to the action functional and enforced through Lagrange multipliers. The key constraint equations utilized in the derivations are the volume fraction constraint and the material form of conservation of mass. When considering finite deformations, the volume fraction constraint must be enforced in the deformed configuration which might require pull-back operations to the reference configuration. Pull-back operations have not been well-developed in the context of peridynamic mechanics. Likewise, the material form of conservation of mass in the classical theory utilizes the determinant of the deformation gradient, the Jacobian determinant, to described the volume scaling between the reference and deformed configurations. In peridynamic theory, the displacement field can be discontinuous and therefore the deformation gradient is potentially undefined. Additionally, in the modeling of solid materials, the peridynamic pressure at a material point is considered to be a function of the totality of deformation within a nonlocal region of the point. This implies that the material points density is influenced nonlocally as well, i.e. a nonlocal conservation of mass. Therefore, we propose a "peridynamic Jacobian determinant" that represents the volume scaling of the nonlocal interaction region between the reference and deformed configurations. In this work we present an efficient tensor measure to compute this peridynamic Jacobian determinate and it's Frechet derivative. Additionally, we present nonlocal tensor analogues of the left- and right-Cauchy Green deformation tensors and show how they can be used in pull-back operations and constitutive modeling of peridynamic materials. Finally, we develop finite deformation conservation of momentum equations for a two-specie peridynamic mixture that is in analogy with classical poromechanics.

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Title: A Plasticity Model for Fiber-Reinforced Geomaterials

Author(s): *Craig Foster, *Univ. of Illinois at Chicago*; Persid Koci, *University of Iliinois at Chicago*.

Geomaterials such as rock, soil, and concrete are typically weak and fairly brittle in tension, limiting the application and, in some situations, durability. In structural applications, tensile strength and ductility can be quite important. Of the several approaches for improving tensile performance, fiber reinforcement has shown much promise. In this research, we focus on fiber reinforcement of cement-stabilized rammed earth using natural fibers, particularly coir fiber. The cement stabilization imparts extra cohesive strength that added to any standard soil plasticity model. The fiber model is built up by initially examining the behavior of individual fibers. While there is some variation in the strength of individual coir fibers, tension tests are well fit by a linear hardening plasticity model. The failure at the end is sudden, and is modeled by an immediate reduction to zero strength when the peak stress is reached. While this corresponds to zero fracture energy, it is incorporated into the fiber model. Fibers may also slip relative to the matrix in which they are embedded, which also creates a plastic response. The fiber slip model relates the average confining stress on the fiber, friction angle and cohesion between the fiber and matrix to the tension in the fiber direction. These two effects result in one-dimensional multi-surface plasticity model for each individual fiber. The multisurface plasticity model for each fiber is integrated over the half unit sphere (since if v is a fiber direction, so is –v) corresponding to the probability density that fibers are oriented in that particular direction. The orientation integration is approximated by a weighted sum over the orientations. This model for the bulk fiber contribution is weighted by the volume fraction of fibers and coupled with a model for the bulk matrix. We begin by using a simple Drucker-Prager model for the matrix, but more sophisticated models are possible. The model is verified in cases of pure fiber fracture and slippage, and the model is then compared to experimental tests of fiber-reinforced rammed earth.

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Title: Higher-Order Conformal Decomposition Finite Element Method (CDFEM) as an Alternative for XFEM

Author(s): *Thomas-Peter Fries, *Graz University of Technology*.

It is well-known that higher-order accurate results with the XFEM are not easily achieved, in particular in the context of interface problems [1]. This may be traced back to the enrichments which are not always able to reproduce independent polynomials on both sides of an interface plus additional (continuity) constraints. Also the integration in cut elements is a challenging task in higher-order XFEM, especially in three dimensions. Herein, we follow the path of the conformal decomposition FEM (CDFEM) as proposed in [2] and extend this to higher-order accuracy. Starting point is a higher-order background mesh where level-set data at the nodes imply internal boundaries and interfaces. Background elements which are cut by the zero-level sets are decomposed into conforming sub-elements. This follows a two-step procedure where, firstly, the zero-level sets are detected and meshed by surface elements (reconstruction) and, secondly, split into sub-elements on the two sides depending on the cut situation (decomposition). It has been shown in [3] that this generation of elements is also useful for the reliable integration in higher-order XFEM but, here, these elements are used in a classical FEM-sense. Node manipulations of the background mesh ensure that the resulting elements are shape-regular. Adaptivity is an important ingredient of the proposed method to ensure robust and efficient results. Numerical results are presented in two and three dimensions and confirm that optimal, higher-order convergence rates are achieved in applications typical for the XFEM and fictitious domain methods. [1] K.W. Cheng, T.P. Fries: Higher-order XFEM for curved strong and weak discontinuities, Internat. J. Numer. Methods Engrg., 82, 564-590, 2010. [2] D.R. Noble, E.P. Newren, J.B. Lechman: A conformal decomposition finite element method for modeling stationary fluid interface problems, Internat. J. Numer. Methods Engrg., 63, 725-742, 2010. [3] T.P. Fries, S. Omerovi■, D. Schöllhammer, J. Steidl: Higher-order meshing of implicit geometries—part I: Integration and interpolation in cut elements, Comp. Methods in Appl. Mech. Engrg., 313, 759-784, 2017.

14th U.S. National Congress on Computational Mechanics
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Title: Shock Wave-Free Interface Interaction

Author(s): *Roman Frolov, Rouslan Krechetnikov, *University of Alberta*; Peter Minev, *University of ALberta*.

The goal of the study is to develop an efficient numerical algorithm applicable to a wide range of compressible flows and use it to enhance the physical understanding of a shock wave refraction at a fluid-fluid interface. The latter problem has been widely studied using experimental, analytical, and numerical techniques. While various physical effects and possible interaction patterns for different geometries have been identified in the literature, the effects of viscosity and surface tension are usually neglected in such models. We also use code based on this numerical algorithm to study such phenomena and their influence on the flow structure of the shock-interface interaction. The proposed method combines a novel algorithm for hyperbolic conservation laws by Guermond and Popov [1], massively parallelizable direction splitting of the viscous stress tensor, designed for the compressible flow case, an interface-capturing technique with surface tension treatment and an interface sharpening procedure. An asymptotic analysis of low Mach number limit has been performed to reveal the typical issues experienced by shock-capturing schemes in the incompressible limit due to the scaling of the artificial viscosity term as Mach number approaches zero. A special fix has been proposed to overcome the issues and ensure the ability of the algorithm to compute flows with low Mach number regions. The capabilities of the algorithm are demonstrated by the wide range of numerical tests representing different physical phenomena. Finally, the method is used to analyze the physics of a shock wave refraction at an interface in presence of viscosity and surface tension. References: [1] J.-L. Guermond and B. Popov, "Invariant domains and first-order continuous finite element approximation for hyperbolic systems", https://arxiv.org/pdf/1509.07461.pdf

14th U.S. National Congress on Computational Mechanics
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Title: Optimization of Origami Crease Topology through Cellular Division

Author(s): *Kazuko Fuchi, *University of Dayton Research* ; Marcelo Kobayashi, *University of Hawaii at Manoa*; Andrew Gillman, *UES, Inc.*; Edward Alyanak, Philip Buskohl, *Air Force Research Laboratory*.

Origami design concepts have been demonstrated to increase the functionality for many engineering applications. An origami design paradigm additionally offers manufacturing advantages, as designs are planned, patterned and initially assembled in a flat configuration, but can access multiple, complex 3D folded states once deployed. The richness of the design space offered by origami, and its attending complex relationship between design and engineering function, motivates the development of robust design methods that guide the selection of an optimal crease topology. In this work, we propose the use of engineered biomimicry for origami design. Our previous work for mechanism design used gradient-based optimization to distribute fold stiffness along candidate fold lines within a prescribed reference grid to select a locally optimal origami crease topology [1]. However, the choice of the reference grid constrains the space of accessible fold topologies and biases the design space explored. To address this limitation, we introduce a map L-system approach for grid generation to broaden the diversity of fold topologies available for the design. An L-system is a formal parallel rewriting system developed by theoretical biologist Lindenmayer [2], who described plant growth strategies through a set of production rules. The map L-system is a variation of the latter that models cellular division, and its use for structural topology optimization problems was introduced by Pedro and Kobayashi [3]. We draw parallels between production rules and origami design strategies. The production rules are encoded in a binary string that represents a gene and are optimized using a genetic algorithm. Each gene is interpreted using a map L-system and translated into an origami reference grid, which is then evaluated for its use in a mechanism design. A few cycles of the gradient-based optimization is applied to all designs to exploit its neighborhood in the design space. A few selected designs that survive through generations have these cycles continued until convergence. The present work introduces a formulation to use a map L-system for origami design for the first time. [1] K. Fuchi et al., "Origami actuator design and networking through crease topology optimization," Journal of Mechanical Design, 137(9), p. 091401, 2015. [2] P. Prusinkiewicz and A. Lindenmayer, The algorithmic beauty of plants. Springer Science & Business Media, 2012. [3] H. T. C. Pedro and M. H. Kobayashi, "On a cellular division method for topology optimization," International Journal for Numerical Methods in Engineering, 88(11), pp. 1175-1197, 2011.

14th U.S. National Congress on Computational Mechanics
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Title: A Numerical Tornado Model Unifying the Existing Experimental Tornado Simulators

Author(s): *Anant Gairola, *Western University*; Zoheb Nasir , Girma Bitsuamlak, *Western University* .

The current state of the art in studying tornado-like vortices at engineering scale (which is to be differentiated from meteorological scale) dictates the use of mechanically driven vortices in experimental simulators. However, the differences in the mechanisms utilized to produce these vortices and the physical limitations of measuring various characterizing parameters of a tornado-like vortex (aspect ratio, swirl ratio etc.) in an experimental set up, often lead to misinterpretation of results and makes these results very specific to the experimental set-up. The present study develops a numerical simulator, that unifies the existing simulators and facilitates a universal interpretation. In this study, VorTECH at Texas Tech University, Tornado Simulator at Iowa Sate University (ISU) and WindEEE Dome at Western University, are chosen as representatives of “Ward” type, “top-down” type and “3D wind chamber” type simulators, respectively. In the initial validation phase, each simulator is numerically modeled without any simplification (or modification) and placed in a bigger computational domain to simulate their placement in a lab environment with a closed-circuit flow. Once the flow field and pressure profiles are validated with the ones obtained from the original experimental simulators, the relevant boundary conditions are extracted to allow some degree of modification to these models, resulting in simplified and open-circuit CFD models during the second stage of the study. The simplifications are applied to the original simulators, while preserving their respective vortex generation mechanisms, and these simplified models are then used to simulate tornado-like vortices with different values of the characterizing parameters. The analysis of the results leads to a single simplified numerical simulator, which could still be linked to the experimental simulators using a unique calibration scheme. Thus, a numerical simulator is obtained that could (i) link the interpretation of results between the various experimental simulators, and (ii) produce preliminary tornado design parameters numerically. Keywords: Tornado-like vortices, CFD, numerical simulator, boundary conditions, experimental simulator.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Higher Order Homogenization for Piezoelectric Periodic Composites

Author(s): Andrea Bacigalupo, *IMT Lucca*; *Luigi Gambarotta, *University of Genova*.

The analysis of piezoelectric materials having periodic microstructure is carried out through a multi-scale approach based on higher order asymptotic homogenization. It is well known that non-local approaches in piezoelectricity related to internal lengths have been applied both in Fracture Mechanics [1] and when size effects cannot be ignored, as it happens in the analysis of dispersive wave propagation and when high strain and stress gradients are imposed. The material periodicity allows to face the problem with reference to the periodic cell characterizing the material. In this regard, the governing equations at the microscale are reformulated through an asymptotic expansion of the coupled microscopic fields, i.e. the displacement and the electric potential field, so obtaining a sequence of recursive PDE problems. These problems are defined by imposing the solvability condition in the class of periodic perturbations in the unit cell via Fichera's Theorem. From this sequence of problems, the downscaling law is obtained together with averaged infinite order equations [2]. Moreover, to obtain a consistent higher order homogenization, a variational approach involving the electric enthalpy is proposed (as generalization of the approach proposed in [3]) and the governing equation of the higher order continuum is obtained together with the overall constitutive tensors. It is worth to note that the structure of the downscaling law relation and of the overall constitutive tensors are determined in closed form. On the contrary, the perturbation functions involved in such procedure must be obtained through the computational solution of the above defined cell problems. Because the material inhomogeneity in the cell problems the source terms of the PDE problem are singular at the interfaces between the different phases. References [1] Zhou, Z. G., Wang B., The scattering of harmonic elastic anti-plane shear waves by a Griffith crack in a piezoelectric material plane by using the non-local theory, International Journal of Engineering Science, 40, 303-317, 2002. [2] Fantoni, F., Bacigalupo, A., Paggi, M., Multi-field asymptotic homogenization of thermo-piezoelectric materials with periodic microstructure, submitted https://arxiv.org/abs/1701.03361, 2017. [3] Bacigalupo A., Gambarotta L., Second-gradient homogenized model for wave propagation in heterogeneous periodic media, International Journal of Solids and Structures, 51, 1052–1065, 2014.

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Title: A Two-Node Beam Element by Using Isogeometric Approach

Author(s): *Buntara Sthenly Gan, *Nihon University*.

A study on the development of a two-node beam element is presented here. The two-node beam element is developed by using the isogeometric approach based on Euler-Bernoulli or Timoshenko beam theory, which allows the transverse shear deformation and rotatory inertia effect. The natural shape of the beam curvature and the shape functions formulation of the element were developed by following the isogeometric approach formulation. In the isogeometric approach, the number of equations increased according to the number of control points adopted. In this study, a new double condensation method is introduced to reduce the number of equations due to the increasing of control points so that it becomes a conventional two-node beam element. There are two folds of benefit by reducing the degree of freedom to a standard two-node beam element: first, the computation cost is lowered; second, allow a seamless integration into the existing FEM codes. From the numerical results, it is concluded that the present two-node beam element formulation can produce very accurate values in the element stiffness and mass matrices. Finally, the versatility of the current approach was highlighted.

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Title: Numerical Modeling of Void Coalescence and Shear Localization in Ductile Solids

Author(s): *Xiaosheng Gao, Tuo Luo, *University of Akron*.

Ductile fracture has been attributed to a process of void nucleation, growth and coalescence under the triaxial stress state and a process due to shear localization when the stress triaxiality becomes low. Detailed finite element analysis of a representative material volume has shown to be an effective method to study material failure mechanism and to identify parameters controlling the ductile fracture process. Previous studies suggest the final material failure process is localized into a narrow band while material adjacent to this band undergoes elastic unloading. This facilitates a numerical model consisting of three layers of materials. By conducting a systematic analysis of the representative material volumes subjected to various stress states, this study discusses different failure mechanisms, such as void growth, void collapse and shear localization, examines several existing failure criteria, and proposes a localization criterion based on the interaction between the three layers of material. Among the discussed failure mechanisms, necking of the material between collapsed voids at the later stage of loading is found to cause reopening of voids and leads to material failure at low stress triaxialities. Finally a ductile failure criterion in terms of strain to failure as a function of the stress triaxiality and the Lode parameter is established.

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Title: An Efficient Method for Transient Heat Conduction in Periodic Structures

Author(s): *Qiang Gao, *Department of Engineering Mech*; Haichao Cui, Ying Feng, *Department of Engineering Mechanics, Faculty of Vehicle Engineering and Mechanics, Dalian University of Technology*.

An efficient and accurate method is proposed for solving transient heat conduction in periodic structures. Based on the physical features of transient heat conduction, the periodic property of the structure and the physical meaning of the matrix exponential, the sparsity of the matrix exponential corresponding to the periodic structures and the repeatability of the elements in the matrix are proved in this paper. According to the algebraic structure of the matrix exponential and the precise integration method (PIM), an efficient and accurate method is proposed by computing the matrix exponential corresponding to a representative periodic structure (RPS) with a few unit cells instead of computing the matrix exponential corresponding to the entire periodic structure. The proposed method can avoid computing and sorting many zero elements and identical elements. Therefore, the proposed method is more efficient and requires less memory. Simultaneously, the proposed method inherits the accuracy and stability of the original PIM. Numerical examples show that the proposed method can obtain accurate solutions even with a larger time step and that the proposed method is significantly more efficient than the Crank-Nicholson method.

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Title: Numerical Simulation of Natural Convection Heat Transfer in a Heat Exchanger Using an Incompressible Smoothed Particle Hydrodynamics (SPH)

Author(s): *Faroogh Garoosi, Ahmad Shakibaeinia, *École Polytechnique de Montréal*.

An incompressible smoothed particle hydrodynamics (SPH) model is developed and evaluated for study of natural convection heat transfer in a heat exchanger containing a pair of hot and cold. Natural convection fluid flow and heat transfer in two different benchmark enclosures (i.e., differentially heated cavity and L-shaped enclosure) are used as a validation case. Validations show the comparability of simulation results of the present SPH model and those obtained based on the mesh-based methods. A parametric study is also done to explore the effects of the pertinent parameters such as: Rayleigh number and orientation of the hot and cold cylinders on the thermal performance of the heat exchanger. Results are presented in terms of isotherms, velocity streamlines, and the average Nusselt number. The presented results reveal that heat transfer rate and maximum values of stream function increase with the increment of the Rayleigh number. Finally, it is found that, orientation of the hot and cold cylinders plays a significant role on the flow and thermal fields within the enclosure.

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Title: Convergence of Adaptive FEM for the Approximation of Eigenvalues of PDEs in Mixed Form

Author(s): *Lucia Gastaldi, *Università di Brescia*.

The design of a strategy for adaptively computing the finite element approximation of eigenfunctions of partial differential equation, can be a difficult task in presence of multiple eigenvalues or clusters of eigenvalues. In this talk we present the convergence and quasi-optimality analysis for the approximation of Laplace eigenvalue problem in mixed form. Our analysis is based on a properly defined a posteriori error estimator and covers the discretization by means of Raviart-Thomas or Brezzi-Douglas-Marini families of mixed finite elements. We review briefly a priori and a posteriori error estimates and discuss how the theory applies in presence of multiple eigenvalues or clusters of eigenvalues (joint work with D. Boffi, D. Gallistl, and F. Gardini). The analysis for mixed Laplacian suggests how to define an error indicator for the eigenvalues of Maxwell's system. For this indicator we can prove reliability and efficiency (joint work with D. Boffi, R. Rodriguez, and I. Sebestova).

14th U.S. National Congress on Computational Mechanics
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Title: Large-Scale Real-Space Electronic Structure Calculations

Author(s): *Vikram Gavini, Phani Motamarri, *University of Michigan*.

In this talk, the development of a real-space formulation for Kohn-Sham density functional theory (DFT) and a finite-element discretization of this formulation [1,2], which can handle arbitrary boundary conditions and is amenable to adaptive coarse-graining, will be presented. In particular, the accuracy afforded by using higher-order and enriched finite-element discretizations, and the efficiency and scalability of the Chebyshev filtering algorithm in pseudopotential and all-electron Kohn-Sham DFT calculations will be demonstrated. Further, the development of a subquadratic-scaling approach (in the number of electrons) based on a subspace projection and Fermi-operator expansion will be discussed [3], which will be the basis for the development of quasi-continuum coarse-graining techniques for Kohn-Sham DFT. The developed techniques have enabled, to date, pseudopotential calculations on ~10,000 atoms, as well as all-electron calculations on systems containing ~10,000 electrons. [1] P. Motamarri, M.R. Nowak, K. Leiter, J. Knap, V. Gavini, Higher-order adaptive finite-element methods for Kohn-Sham density functional theory, J. Comp. Phys. 253, 308-343 (2013). [2] B. Kanungo, V. Gavini, Large-scale all-electron density functional theory calculations using an enriched finite element basis, Phys. Rev. B 95, 035112 (2017). [3] P. Motamarri, V. Gavini, A subquadratic-scaling subspace projection method for large-scale Kohn-Sham DFT calculations using spectral finite-element discretization, Phys. Rev. B 90, 115127 (2014).

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Title: A Novel Hybrid Additive/Multiplicative Schwarz Preconditioner for Monolithic Solvers of Surface-Coupled Multiphysics Problems

Author(s): *Michael Gee, Maximilian Noll, Matthias Mayr, *TU Munich*.

We propose a hybrid additive/multiplicative Schwarz preconditioner for the monolithic solution of surface-coupled problems. Powerful preconditioning techniques are crucial when it comes to solving large monolithic systems of linear equations efficiently, especially when arising from coupled multi-physics problems like in fluid-structure interaction. Existing physics-based block preconditioners have proven to be very powerful, but accumulate the error at the coupling surface. We address this issue by combining them with an additional additive Schwarz preconditioner, whose subdomains span across the interface on purpose. By performing cheap but accurate subdomain solves that do not depend on the separation of physical fields, this error accumulation can be reduced effectively. Extensive numerical experiments compare the performance of the different preconditioners and demonstrate the increased efficiency and scalability of the proposed approach up to a large number of unknowns and cores.

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Title: An Optimization Based Phase Field Model for Continuous-Discontinuous Fracture

Author(s): *Rudy Geelen, Yingjie Liu, John Dolbow, *Duke University*.

The present study concerns the development of a framework unifying diffuse and sharp interface models of fracture. Diffuse interface models, e.g. phase field, have received considerable attention because of their ability to deal with numerous bifurcation and coalescence events. On the other hand, inserting a strong discontinuity circumvents excessive mesh distortion and avoids the need of a stability parameter to maintain well-posedness. Recently, attempts have been made to transition between continuous and discontinuous models of fracture using complex geometric algorithms [1, 2]. However, these approaches involve a cumbersome implementation and have yet to demonstrate robustness in an evolving interface problem. We propose a method attempting to unify continuous and discontinuous fracture models by means of a phase field based optimization algorithm. Phase field models for brittle fracture allow for a closed-form solution for the damage field in a one-dimensional setting. This idea can be extended to hold for two and three spatial dimensions in the form of a signed distance function. In an effort to address complex fracture problems, the framework was enhanced with a geometric skeletonization operation over a regular grid on top of the computational domain. This procedure involves identifying the different cracks, parameterizing their topologies and creating an initial guess for the numerical optimization algorithm. The proposed framework is demonstrated to perform well both for single cracks as well as for more complex fracture problems. Because this continuous-discontinuous fracture model is defined in the form of an optimization problem, results are quasi-independent from the quality of the superimposed grid. As the optimization algorithm works with analytical solutions, the resulting framework can be seamlessly incorporated in any evolving interface problem with a minimal increase in computational expense and virtually no heuristics. Keywords: continuous-discontinuous strategy, crack propagation, fracture mechanics, phase field models,discontinuity detection, optimization References: [1] Elena Tamayo-Mas and Antonio Rodr ■■guez-Ferran. A medial-axis-based model for propagating cracks in a regularised bulk. International Journal for Numerical Methods in Engineering, 101(7):489–520, 2015. ISSN 1097-0207. [2] Vahid Ziaei-Rad, Li Shen, Jiahao Jiang, and Yongxing Shen. Identifying the crack path for the phase field approach to fracture with non-maximum suppression. Computer Methods in Applied Mechanics and Engineering, 312:304–321, 2016.

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Title: Accurate Phase-Field Solution of Sneddon's Problem: Main Ingredients and Challenges

Author(s): *Tymofiy Gerasimov, Laura De Lorenzis, *TU Braunschweig, Germany*.

The fundamental role of crack-tip asymptotic exponents (1/2, 2/3 and 5/8) for different hydraulic fracture propagation regimes (resp., toughness, leak-off and viscosity dominated ones) and their interplay is widely acknowledged [1]. Recent and quite intensive attempts to incorporate the fracture phase-field modelling framework [2] into the hydraulic fracture formulations [3,4] and, in particular, to clarify its ability to accurately reproduce and capture the corresponding asymptotes are, to the best of our knowledge, not yet conclusive. We address this by revisiting the quasi-static Sneddon-Lowengrub benchmark with a classical square root crack opening displacement. We study the effect of the three major ingredients of the phase-filed formulation of (brittle) fracture -– (i) the type of tension-compression split of the stored elastic energy density function, (ii) the choice of a specific polynomial function constituting the local part of the dissipated density due to fracture, and, finally, (iii) the form of crack irreversibility constraint –- onto the finite element solution accuracy, as well as efficiency. [1] E.V. Dontsov, A.P. Peirce. A multiscale Implicit Level Set Algorithm (ILSA) to model hydraulic fracture propagation incorporating viscous, toughness and leak-off asymptotics. Comput. Methods Appl. Mech. Eng. 313 (2017), 53-84. [2] M. Ambati, T. Gerasimov, L. De Lorenzis. A review on phase-field models of brittle fracture and a new fast hybrid formulation. Comput. Mech 55 (2015), 383-405. [3] Z.A. Wilson, C.M. Landis. Phase-field modeling of hydraulic fracture. J. Mech. Phys. Solids 96 (2016) 264-290. [4] S. Lee, M.F. Wheeler, T. Wick. Iterative coupling of flow, geomechanics and adaptive phase-field fracture including level-set crack width approaches. J. Comp. Appl. Math. 314 (2017) 40-60.

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Title: PUMA (Polyhedra Unstructured Mesh Adaption): A Novel Method to Refine and Coarsen Convex Polyhedra

Author(s): *Thomas Gessner, Sandeep Menon, *Ansys Inc.*.

Mesh adaption techniques are used widely in academic and commercial simulation software to locally or globally refine and subsequently coarsen meshes, as it provides the means to achieve higher solution accuracy with a marginal increase in computational expense. Polyhedral meshes are particularly attractive because they can be used to accurately represent various geometries being modeled, while providing considerable flexibility with regard to mesh generation. The algorithms developed over the past 30 years, e.g. [1], [2], are limited to meshes with standard element types, i.e. hexahedra, tetrahedra, prisms, and pyramids in 3D, quadrilaterals, triangles in 2D. In contrast, the PUMA (Polyhedra Unstructured Mesh Adaption) method can refine all these standard element types and is additionally able to refine convex polyhedra elements. Polyhedra are significantly more difficult to refine because of their arbitrary shape. There are no templates that can be used to query the connectivity between faces and nodes e.g. to find out which faces of the polyhedra are adjacent to a given face or which nodes are connected via an edge to a given node. Templates that provide this information are readily available for standard element types but for polyhedra, the local connectivity in each element needs to be constructed to enable such queries. In PUMA the standard element types are simply considered as polyhedra and the method thus unifies adaption of all element types. The parallel implementation of PUMA is integrated in the finite volume CFD software ANSYS Fluent, where it is combined with dynamic load balancing to keep an equal load on all compute nodes and to prevent memory spikes on individual compute nodes during the adaption process. A wide range of examples demonstrates the capabilities of PUMA to - Adapt polyhedra and standard elements while maintaining the mesh quality, - Dynamically refine and subsequently coarsen meshes for steady-state and transient problems, - Provide a tool to efficiently resolve flow features on meshes of any type. [1] M.C. Rivara. Algorithms for refining triangular grids suitable for adaptive and multigrid techniques. Int. J. Numer. Methods. Eng., 20:745-756, 1984. [2] M.J. Berger, P. Colella. Local adaptive mesh refinement for shock hydrodynamics. J. Comput. Phys., 82:64-84, 1989.

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Title: Polynomial Chaos for the Multiscale Characterization of Material Response and Failure under Uncertainty

Author(s): Loujaine Mehrez, *Roger Ghanem, *USC*; Venkat Aitharaju, William Rodgers, *GM Corp*.

We describe a comprehensive and numerically tractable approach for characterizing material response including failure under conditions of multiscale coupling and multiscale uncertainty. The proposed approach expresses quantities of interest (elastic, inelastic, or failure properties) at any scale as function of uncertainties and parameters from finer scales. Modeling errors associated with upscaling procedures are also accounted for and included both in the propagation, estimation, and updating procedures. The construction of the polynomial chaos expansion can be accomplished with any amount of available information, acquired on any of the relevant scales. We demonstrate the applicability of this methodology to the problem of characterizing the properties and performance of composite materials for use in design optimization under uncertainty.

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Title: A Deep Learning-Based Constitutive Model for Finite Element Method

Author(s): *Fariborz Ghavamian, Angelo Simone, *Faculty of Civil Engineering and Geosciences, Delft University of Technology*.

Developing physics-based constitutive models for materials with complex behavior, such as polymers and composites, is a complicated and error-prone task. Complex because the underlying physics of these materials is usually not fully understood; prone to error because the experimental data are often unreasonably idealized to allow fitting with a restrictive physic-based model. In this contribution, we investigate a Deep Learning-based constitutive model and employ it in the framework of the Finite Element Method (FEM). The Deep Learning model is fundamentally dependent on experimental data and therefore it does not suffer from restrictiveness of a physics-based model. Technically, (i) we develop a Recurrent Neural Network to capture the path-dependent behavior of the material; (ii) we employ prediction intervals to measure the degree of confidence in predictions of the model; (iii) we propose an automatic differentiation technique to compute the consistent tangent of a Deep Learning constitutive model with an arbitrary number of hidden layers. The proposed model is trained on artificially generated data. The fundamental characteristics of the data distribution are strain-softening and path-dependency. To overcome the mesh-sensitivity of the FEM model, which is an artifact of the strain-softening constitutive model, we employ a gradient-enhanced computational framework.

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Title: Nonlinear Dynamics and Pull-In of Microplate-Based MEMS

Author(s): *Mergen Ghayesh, *University of Adelaide*; Hamed Farokhi, *McGill University*.

Low fabrication cost and energy consumption as well as high performance are the main reasons behind the high-speed growth in the application of microelectromechanical systems (MEMS) in engineering systems such as in sensors and actuators, micro energy harvesters, and airbag accelerometers. Microplates are the common deformable electrodes of electrically actuated MEMS; the oscillation/deformation response of these microstructures is the operation principle in many MEMS. Nonlinear dynamics and pull-in characteristics of an imperfect microplate-based MEMS are investigated, for the first time, via mathematical modelling and numerical simulations. The influence of the small-size is incorporated via the modified couple stress theory. All the transverse and in-plane inertia and displacements are considered via the von Kármán nonlinear theory and the Kirchhoff hypothesis. A combination of DC and AC voltages are applied to the deformable electrode of a fully-clamped microplate type. The electrical-field loading, the kinetic energy, the size-dependent potential energy, and damping effects are related by means of the Lagrange equations which yields the mathematical model of the microsystem involving displacement/electrical nonlinearities in the oscillation model. The backward differentiation formula (BDF) coupled with a parameter-continuation method is used for the nonlinear numerical simulations. In the absence of the AC voltage, the electrostatic pull-in and bending deflection are analysed by increasing the DC polarisation voltage. The effects of the imperfection and being small of the order of 10 through -6, on the pull-in, are also highlighted. The AC frequency-oscillation characteristics of the electrically actuated microsystem are also analysed when subject to both the DC and AC voltages, by analysing snap-through motions and jump phenomena.

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Title: Static Analysis of Sandwich Beams Including the Effect of Adhesive Layers by Using the Mixed Refined Zigzag Theory

Author(s): *Marco Gherlone, *Politecnico di Torino, Italy*.

Sandwich laminates are used in several engineering fields, ranging from aircraft and naval to civil structures. Their success is due to the high stiffness-to-weight ratio (related to low-density core), to the impact energy absorption capacity and to the thermal and acoustic insulation properties. Modelling sandwich structures is challenging due to their inherent transverse anisotropy (stiff facesheets and deformable core) and to the complex core geometry (honeycomb, corrugated, cellular). Moreover, experimental investigation on adhesively bonded sandwich structures have revealed that structural deterioration starts at the interface between the core and the facesheet [1]. Adhesive layers should be included in an accurate analysis of sandwich structures in order to accurately predict damage modes. Among the several approaches for the analysis of laminated composite and sandwich structures, zigzag theories represent an interesting trade-off between accuracy and computational cost. Belonging to this class, the Refined Zigzag Theory (RZT) has been recently proposed [2]. RZT has shown to be accurate for a wide range of applications (global and local static response, natural frequencies, buckling loads) and material systems (including sandwich structures with traditional and functionally graded layers). A further development of RZT is RZT(m) which improves the transverse shear stress and strain prediction by adopting Reissner's mixed variational theorem [3]. The accuracy of RZT(m) is remarkable even in presence of very thin and compliant layers [3]. This capability makes RZT(m) a good candidate for the modelling of the adhesive layers of sandwich structures. Aim of this work is to investigate, using RTZ(m), the effect of modelling sandwich beams by taking into account the adhesive layers. The theory will be reviewed and the computational framework for the numerical investigation will be set. Both analytical and finite element solutions will be used to provide the static response prediction of sandwich beams under typical loading conditions. The accuracy of the RTZ(m) results will be assessed by comparison with other approaches [1], exact-elasticity solutions (when available) or high-fidelity FE model based on commercial codes. [1] S.J. Huang, An analytical method for calculating the stress and strain in adhesive layers in sandwich beams, Composite Structures 60, 105-114, 2003 [2] A. Tessler, M. Di Sciuva and M. Gherlone, A refined zigzag beam theory for composite and sandwich beams, Journal of Composite Materials 43(9), 1051-1081, 2009 [3] A. Tessler, Refined zigzag theory for homogeneous, laminated composite, and sandwich beams derived from Reissner's mixed variational principle, Meccanica 50(10), 2621-2648, 2015

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Title: Computational Framework Involving Spatial and Temporal Multi-Scaling for Coupled Transient Electromagnetics-Mechanical Phenomena

Author(s): *Somnath Ghosh, Shu Guo, Reza Yaghmaie, *Johns Hopkins University*.

Multi-functional devices that integrate electromagnetic and mechanical fields are gaining importance in a wide variety of applications. The combined mechanical and electromagnetic regimes, encompassed in these structures, make it necessary to develop effective multi-physics analysis tools at a range of temporal scales. This work develops a framework for coupling transient electromagnetic (EM) and dynamic mechanical (ME) fields to predict the evolution of electrical and magnetic fields and their fluxes in a vibrating substrate undergoing finite deformation [1]. To achieve coupling between fields the governing equations are solved in the time domain. A Lagrangian description is invoked, in which the coupling scheme maps Maxwell's equations from spatial to material coordinates in the reference configuration. Physical variables in the Maxwell's equations are written in terms of a scalar potential and vector potentials. Non-uniqueness in the reduced set of equations is overcome through the introduction of a gauge condition. An important consideration is that the different fields governing multi-physics response may have large frequency discrepancies, e.g. the ultra-high electromagnetic frequencies and moderate vibration frequencies. Computational analyses of these discrepant frequency problems using conventional time integration schemes can become intractable. This work addresses the issue of time integration with large frequency ratios, by introducing a novel wavelet transformation induced multi-time scaling (WATMUS) method in the finite element framework. The method significantly enhances the computational efficiency in comparison with conventional single time scale integration methods. An adaptive enhancement of WATMUS scheme allows for the optimal wavelet bases in the transformation and integration step sizes. The accuracy and efficiency of the proposed WATMUS scheme is verified by comparing the results with the single time-scale simulations of the coupled transient electromagnetic nonlinear vibration problems. [1] S. Guo and S. Ghosh, Comp. Mech., 2014. [2] R. Yaghmaie, S. Guo and S. Ghosh, Comp. Meth. Appl. Mech. Engng., CMAME, 2016.

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Title: Computational Framework Involving Spatial and Temporal Multi-Scaling for Coupled Transient Electromagnetics-Mechanical Phenomena

Author(s): *Somnath Ghosh, Shu Guo, Reza Yaghmaie, *Johns Hopkins University*.

Multi-functional devices that integrate electromagnetic and mechanical fields are gaining importance in a wide variety of applications. The combined mechanical and electromagnetic regimes, encompassed in these structures, make it necessary to develop effective multi-physics analysis tools at a range of temporal scales. This work develops a framework for coupling transient electromagnetic (EM) and dynamic mechanical (ME) fields to predict the evolution of electrical and magnetic fields and their fluxes in a vibrating substrate undergoing finite deformation [1]. To achieve coupling between fields the governing equations are solved in the time domain. A Lagrangian description is invoked, in which the coupling scheme maps Maxwell's equations from spatial to material coordinates in the reference configuration. Physical variables in the Maxwell's equations are written in terms of a scalar potential and vector potentials. Non-uniqueness in the reduced set of equations is overcome through the introduction of a gauge condition. An important consideration is that the different fields governing multi-physics response may have large frequency discrepancies, e.g. the ultra-high electromagnetic frequencies and moderate vibration frequencies. Computational analyses of these discrepant frequency problems using conventional time integration schemes can become intractable. This work addresses the issue of time integration with large frequency ratios, by introducing a novel wavelet transformation induced multi-time scaling (WATMUS) method in the finite element framework. The method significantly enhances the computational efficiency in comparison with conventional single time scale integration methods. An adaptive enhancement of WATMUS scheme allows for the optimal wavelet bases in the transformation and integration step sizes. The accuracy and efficiency of the proposed WATMUS scheme is verified by comparing the results with the single time-scale simulations of the coupled transient electromagnetic nonlinear vibration problems. [1] S. Guo and S. Ghosh, Comp. Mech., 2014. [2] R. Yaghmaie, S. Guo and S. Ghosh, Comp. Meth. Appl. Mech. Engng., CMAME, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: Improved Partitioned Element Method for Constructing Higher Order Shape Functions on Arbitrary Polyhedra

Author(s): *Brian Giffin, Mark Rashid, *UC Davis*.

We present an improved reformulation of the "partitioned element method" (PEM): a finite-element-like method in which shape functions are defined on arbitrary polygonal and polyhedral element domains. The method proceeds by partitioning an element into quadrature cells, and allowing the element's shape functions to vary according to a local polynomial defined within each of these cells, resulting in piece-wise polynomial shape functions which are discontinuous at quadrature cell boundaries. The polynomial coefficients defined in each cell are obtained by minimizing a quadratic functional which penalizes discontinuities in the shape functions (and their gradients) across all cell interfaces. Unlike the original method (presented in [1]) which is restricted to piece-wise linear approximants, the present formulation admits polynomials of arbitrary degree, leading directly to higher-order completeness of the shape functions, and improved convergence properties. Numerical results for two- and three-dimensional solid mechanics problems are presented, demonstrating the method's ability to overcome issues pertaining to non-convex elements, geometric degeneracies, and certain forms of element locking phenomena – particularly, those concerning thin elements. References: [1] Rashid M, Sadri A. The partitioned element method in computational solid mechanics. Computer Methods in Applied Mechanics and Engineering 2012; 237–240: 152–165.

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Title: Uncertainty Quantification on a Real Case with TELEMAC-2D

Author(s): *Cedric Goeury, *EDF R&D*.

In this study the software TELEMAC-2D has been used with the OpenTURNS library to quantify the uncertainty on a real hydraulic case. The used approach is based on the chaining of OpenTURNS and TELEMAC-2D using the SALOME platform in order to implement a Monte Carlo-like algorithms. Each uncertain parameter (inlet discharge, friction coefficient for instance) is associated to a statistical distribution (defined using OpenTURNS). A sufficient number of TELEMAC-2D runs are achieved with respect to the pre-defined random entries in order to guarantee the convergence of the studied Monte Carlo-like algorithms. To handle the uncertainty with the Monte-Carlo method, it is important to run a lot of simulations in order to have reliable results. EDF's cluster has been used to run the simulations. A reduced order model built using POD approach is also used for heavy cases. The reduced models gave a huge save in CPU time comparing to the full runs of Telemac2D. MPI library was used for launching and managing the Telemac and the ROM runs. Post-processing of the huge amount of results files is tackled through some Python scripts specifically developed within OpenTURNS. The obtained results are analyzed twofold: On one hand, the effect of variability of random inputs is assessed at some specific points (assumed to be around a fictive nuclear power plant). On the other hand, a global statistical analysis all over the domain is done. A spatial distribution of the mean water depth and its variance is obtained. These results are of utmost importance for dimensioning of protecting dykes. Furthermore, there are very useful when establishing scenarios for flood managing. This work shows that, thanks to the availability of important computer resources and to an optimized software, we are able to consider Monte Carlo uncertainty quantification algorithms for real hydraulic models. This critical conclusion was, even unfaisable dream, couple of years ago.

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Title: Multiphysics Modeling the Urea-Induced Responsive Behavior of the Urea-Sensitive Hydrogel

Author(s): *Kek Boon Goh, Hua Li, Khin yong Lam, *NTU*.

Multiphysics modeling the urea-induced responsive behavior of the urea-sensitive hydrogel K.B. Goh, Hua Li, K.Y. Lam School of Mechanical and Aerospace Engineering, Nanyang Technological University (NTU), 50 Nanyang Avenue, Singapore 639798, Republic of Singapore A notable trait of soft biomaterials is their ability to deform in response to certain external bio-stimuli. Here, a multiphysics model is mathematically developed for the characterization of the urea-sensitive hydrogel in response to the urea cues [1]. To capture the urea-induced deformation of the hydrogel, a novel rate of reaction is formulated with the effect of the surrounding pH coupled with environmental temperature on the immobilized urease, and incorporated accordingly into the model. The model is validated via comparison with the published experimental works, where the hydrogels are subjected to the variation of urease loading, and environmental pH and temperature respectively, in which very good agreements are achieved. After examination with the published experimental data, it is thus confirmed that the model can characterize well the responsive behavior of the urea-sensitive hydrogel subject to the urea stimulus, including the distribution pattern of the electrical potential, pH and displacement of the hydrogel. In future work, the multiphysics model is utilized to get a greater insight into the fundamental mechanism of the smart hydrogel in response to the urea cue for potential application as biosensor. Keywords: Multiphysics model; Urea sensitive hydrogel; Urease; Biosensor; Bioelectrochemistry Reference [1]. Goh, K. B., Hua Li, and K. Y. Lam. "Development of a multiphysics model to characterize the responsive behavior of urea-sensitive hydrogel as biosensor." Biosensors and Bioelectronics (2017).

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Title: Modelling of Mechanical Processes Related to Hydraulic Fracturing

Author(s): *Sergey Golovin, *Lavrantyev Institute of Hydrod*; Alexey Baykin, *Lavrentyev Institute of Hydrodynamics*; Alexander Valov, *Novosibirsk State University*.

Hydraulic fracturing is the process of creating a fracture due to pumping a highly pressurized fluid in a rock formation through a wellbore that is used for intensification of hydrocarbon production. Compared to the classical models of brittle fractures, hydraulic fracture theory describes the fluid flow within the fracture coupled with the fracture opening and propagation, exchange of the fracturing fluid with the pore fluid, influence of the pore pressure on the stresses, etc. In the talk, we present our recent development in the modelling of the hydraulic fracture dynamics in a poroelastic medium. The topics include: a numerical algorithm for a simulation of the planar hydraulic fracture propagation in the Biot poroelastic medium; an analysis of the influence of the pore pressure on the dynamics of the fracture; use of non-stationary processes for the determination of fracture's and reservoir's parameters; estimation of the debit of a multiply fractured horizontal wellbore. The contents of the talk is based on the publications cited below. Publications: [1] Baykin, A.N. and Golovin, S.V. (2016). Modelling of hydraulic fracture propagation in inhomogeneous poroelastic medium. J. Phys.: Conf. Ser., 722, 012003. [2] Baykin, A.N. and Golovin, S.V. (2016). Non-symmetry of a hydraulic fracture due to the inhomogeneity of the reservoir. arXiv:1610.09471 [3] Golovin, S.V. and Gadylshina, K.A. (2016). Fluid flow in a reservoir drained by a multiple fractured horizontal well. arXiv:1602.04041. [4] Golovin, S.V., Isaev, V.I., Baykin, A.N., Kuznetsov, D.S. and Mamontov, A.E. (2015). Hydraulic fracture numerical model free of explicit tip tracking. Int. J. Rock Mech. Min. Sci., 76, 174–181. [5] Golovin, S.V. and Baykin, A.N. (2016). Influence of pore pressure to the development of a hydraulic fracture in poroelastic medium. arXiv:1608.08001. [6] Shelukhin, V.V., Baikov, V.A., Golovin, S.V., Davletbaev, A.Y. and Starovoitov, V.N. (2014). Fractured water injection wells: Pressure transient analysis. Int. J. Sol. Struct., 51(11), 2116–2122. [7] Valov, A.V. and Golovin, S.V. (2016). Determination of hydraulic fracture parameters using a non-stationary fluid injection. J. Phys.: Conf. Ser., 722, 012008.

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Title: Full-Field 4D Measurements of Acceleration-Induced Deformation in the Living Human Brain

Author(s): *Arnold Gomez, Jerry Prince, *Johns Hopkins University*; Andrew Knutsen, Dzung Pham, *Henry Jackson Foundation*; Philip Bayly, *Washington University in St. Louis*.

Traumatic brain injury (TBI) arises from rapid acceleration of the skull and can induce symptoms ranging from momentary loss of consciousness to chronic disabilities. Experimental measurements of brain-skull displacement are fundamental to quantifying the biomechanics of acceleration-induced TBI. We have previously applied tagged magnetic resonance imaging (MRI) to extract measurements of brain deformation at low accelerations in humans in vivo. This information can be used to bridge the knowledge gaps in the mechanisms between deformation-induced disruptions in neuronal tissue at the cellular level, and macroscopic deformation patterns during head-brain acceleration. Using MRI-based deformation measurements, two-dimensional measurements of in-plane strain on slices spanning the whole brain can be computed [1]. However, experimental constraints, such as the need to repeat head motion during MRI acquisitions during a limited scan time, restrict the resolution and consistency of tagging data. Thus, the collection of image slices, on its own, is insufficient to define a complete quantification of deformation (the strain tensor) across three-dimensional space and time. This research introduces novel data collection and processing strategies for deriving accurate, four-dimensional (4-D), full-field measurements of displacement and strain. The acquisition strategy includes specialized hardware, triggering strategies, and pulse sequences for obtaining tagged MRI in human volunteers. Image processing consists of harmonic phase analysis with finite element models (HARP-FE), which enforces mechanical regularization on the results to reduce artifacts and produce a smooth strain field. The analysis pipeline was applied to images from healthy volunteers during non-injurious rotational and linear accelerations, spiking between 2-4 g in magnitude. The resulting displacement fields exhibited patterns consistent with the direction of the acceleration pulse. However, the principal deformation direction (first principal strain axis) exhibited different patterns, including a concentric rotation-like arrangement immediately after the acceleration peak. Maximum shear strains ranged between 2-4%. These preliminary results demonstrate the extraction of dense, full-field, 4-D motion estimates of in vivo brain tissue under acceleration, and underscore the importance of the constitutive and anatomical relationships between the brain and the skull. The presence of rotation-like deformation patterns in the brain may be due to the internal features of the skull and the meningeal connectivity between the skull and brain. Further application of this measurement technology will elucidate the biomechanical response of different brain structures. These data can be used immediately for the validation of computational models of TBI. [1] Bayly, et al. Annu Rev Biomed Eng. 2012; 14: 369–396.

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Title: Advancing Hyperbolic Solutions through Unstructured Meshes by Mapped Tent Pitching

Author(s): *Jay Gopalakrishnan, *Portland State University*.

Many authors have explored ideas to advance numerical solutions of wave and other hyperbolic problems in time through local operations in space time regions. Such methods are naturally high order in both space and time variables whenever the solution is smooth. The ability to advance in time by different amounts at different spatial locations (i.e., local time stepping) distinguishes such schemes. This talk will focus on one such technique where a spacetime domain is progressively meshed by tent shaped objects. The solution can be computed on an unstructured advancing front (and there is no need to maintain entire spacetime data). We present dimension reduction techniques by mapping the equations within a spacetime tent into a form where space and time separates. After detailing techniques based on this mapping, several examples including the acoustic wave equation and the Euler system are considered. This is joint work with Joachim Schoeberl and Christoph Wintersteiger.

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Title: Temperature-Dependent Multi Scale Large Deformation Simulation of Cu-Ag Alloy

Author(s): *Ali Gordan, *corresponding author*; Amir Reza Khoei, *second author*.

In this study, a novel and unprecedented multi-scale hierarchical molecular dynamics (MD) – finite element (FE) coupling method is proposed to demonstrate the influence of temperature on mechanical properties of heterogeneous Nano-crystalline structures. The embedded-atom method (EAM) many-body interatomic potential is implemented to consider pairwise interactions between atoms in the metallic alloys with face-centered-cubic (FCC) lattice structure at different temperatures. In addition, the Nose-Hoover thermostat is employed to adjust the fluctuation of temperature. The atomic nonlinear elastic parameters are obtained via computing second-order derivative of Representative atom's energy and RVE's strain energy density with respect to deformation criterions (deformation gradient and Green strain tensor).Then, the variations of yield stress points and elastic constants are presented for crystal Cu RVE at different concentrations levels of Ag impurities and at various temperatures. To bridge between atomistic and continuum level, the mechanical characteristics are captured in the atomistic level and transferred to the continuum level directly by functions of strains. Furthermore, comparing the numerical results of the present multi-scale method with MD simulation results, discloses that the suggested techniques produce promising results with small amount of error in large deformation, comparing the numerical results of the present multi-scale method with MD simulation results, discloses that the suggested technique produces promising results for evaluating the temperature effects on problems including heterogeneous Nano-crystalline structures. References: [1] Jafarian, N., Temperature-Dependent Multiscale Simulation of Heterogeneous FCC Crystals, in Department of Civil Engineering. 2015, Sharif University of Technology: Kish Island, Iran. [2] Khoei, A.R., F. Jahanbakhshi, and A. Aramoon, A concurrent multi-scale technique in modeling heterogeneous FCC nano-crystalline structures. Mechanics of Materials, 2015. 83: p. 40-65. [3] Davoodi, J., M. Ahmadi, and H. Rafii-Tabar, Molecular dynamics simulation study of thermodynamic and mechanical properties of the Cu–Pd random alloy.

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Title: A Material Point Method for Simulation of Viscoelastic Flows

Author(s): *Peter Gordon, *Exxonmobil Research & Engr.*; Fushen Liu, Holger Meier, Rohan Panchadhara, *ExxonMobil Research & Engr.*; Vikas Srivastava, *ExxonMobil Upstream Research*.

In this presentation we discuss the challenges associated with modeling flows of viscoelastic fluids, and in particular difficulties associated with the high Weissenberg problem, where viscoelastic constitutive models with high levels of elasticity can trigger numerical instabilities in traditional simulation techniques. We introduce a novel simulation technique, based on the Material Point method, capable of capturing many features of polymeric flows observed experimentally. As in the original spirit of the method, material points possess all necessary information about the material constitutive behavior and move with the flow. They are additionally employed as integration points for the Eulerian problem, whose weights are computed as the system evolves in order to ensure exact integration of the discretized conservation equations. We will present a number of examples comparing flows of viscoelastic materials in simple and more complex geometries, comparing to analytical and experimental results to validate the approach, and will show examples of simulation of high-Weissenberg flows where transitions between stable and unstable flow regimes can be directly observed.

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Title: Error Estimation and Adaption in Domain Decomposition Methods

Author(s): *Pierre Gosselet, *LMT (ENS Paris-Saclay/CNRS)*; Valentine Rey, *LSMS (ENAC/EPFL)*; Christian Rey, *SAFRAN TECH*.

Our study takes place in the framework of finite element (FE) and of Domain Decomposition Methods (DDMs), in particular FETI(DP) and BDD(C), which enable one to define robust and scalable parallel iterative solvers. This presentation deals with the computation of guaranteed upper and lower bounds of the error [1]. In addition to a fully parallel computation [3], the proposed bounds separate the algebraic error (due to the use of a DD iterative solver) from the discretization error (due to the FE), which provides an unbiased criterion to stop the iterations. These bounds are also used to improve the goal-oriented error estimation in a substructured context [2]. Assessments on 2D static linear mechanic problems illustrate the relevance of the separation of sources of error and the independence of the bounds with respect to the substructuring. Finally, we steer the iterative solver by an objective of precision on a quantity of interest (qoi). The strategy consists in a sequence of solvings, adaptive local remeshing and recycling of search directions, in order to reach the desired quality for the qoi with minimal computations. References: [1] V. Rey, P. Gosselet and C. Rey. Strict bounding of quantities of interest in computations based on domain decomposition. CMAME, 287(1):212-228, 2015, doi:10.1016/j.cma.2015.01.009. [2] Valentine Rey, Pierre Gosselet, and Christian Rey. Strict lower bounds with separation of sources of error in non-overlapping domain decomposition methods. IJNME, 108(9):1007-1029, 2016, doi:10.1002/nme.5244. [3] A. Parret-Fréaud, V. Rey, P. Gosselet and C. Rey. Improved recovery of admissible stress in domain decomposition methods - application to heterogeneous structures and new error bounds for FETI-DP. IJNME, 2017, doi:10.1002/nme.5462.

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Title: Hydraulic Fracture Simulation

Author(s): *Robert Gracie, Erfan Sarvaramini, *University of Waterloo*; Egor Dontsov, *University of Houston*; Denis Esipov, Sergey Cherny, *Russian Academy of Science*; Anthony Peirce, *University of British Columbia*; Armando Duarte, *University of Illinois Urbana-Champaine*.

The simulation of the hydraulic fracturing (HF) process used during unconventional oil and gas development poses numerous computational and mathematical challenges. In this presentation, we will provide and overview of the physical process of HF used to extract oil and gas from tight formations. Next, we will summarize the main modeling approaches and the advantages and disadvantages of each. Lastly, we will enumerate some open questions in HF simulation to stimulate discussion for the technical presentations of MS301 & MS305.

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Title: Parallel Goal-Oriented Adaptive Inelasticity

Author(s): *Brian Granzow, *RPI*; Assad Oberai, Mark Shephard, *Rensselaer Polytechnic Institute*.

We present an automated approach for goal-oriented error estimation for execution on parallel computers. Goal-oriented error estimation provides a mathematical framework to quantify errors in physically meaningful functional quantities of interest. In general, goal-oriented error estimation consists of three critical steps: solving a primal variational problem, solving a dual variational problem, and localizing error estimates to the mesh entity level. The key feature of the presented approach is the ability to effectively execute these three steps in parallel using a single residual-based code implementation. This approach eliminates the need for tedious and error-prone implementations of linearizations of the primal residual and the functional quantity, which is desirable in the context of inelasticity, where constitutive models and quantities of interest can be highly nonlinear. In this talk, we will discuss how this approach is realized using a variety of packages from the Trilinos software environment and the PUMI parallel mesh services. In particular, the automated solution of the primal and dual variational problems are accomplished via automatic differentiation capabilities provided by Trilinos, the error localization is realized via a recently proposed Partition of Unity method, and the PUMI mesh tools are utilized to drive unstructured mesh adaptation. We will discuss the application of this adaptive goal-oriented error estimation approach to a three dimensional inelasticity example, where a finite deformation, isotropic linear-hardening model with a von Mises yield surface is assumed. We investigate the utility of a variety of quantities of interest, and their utility in the chosen inelasticity example.

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Title: High-Order Polygonal Elements for Elastodynamic Problems

Author(s): *Hauke Gravenkamp, *University of Duisburg-Essen*.

In recent years, polygonal and polyhedral discretizations have gained attention due to their highly flexible meshing capabilities. Numerous approaches have been proposed to formulate interpolations on polygonal topologies. In the context of dynamic simulations at higher frequencies, it is desirable to employ high-order polynomial interpolations, which can significantly reduce the number of nodes per wavelength and lead to exponential convergence rates under p-refinement for smooth problems. However, constructing high-order interpolations on polygonal elements is generally not straightforward. This contribution discusses approaches to derive high-order interpolations based on scaled boundary coordinates. In this coordinate system, as employed in the context of the scaled boundary finite element method, the edges of each polygon are discretized using line elements of arbitrary order, while different analytical and numerical procedures are utilized to describe the behavior of the solution in the interior of the domain. These concepts are employed for elastodynamic problems in the time domain as well as the frequency domain and compared against conventional finite and spectral element formulations. Concepts of constructing polygonal spectral elements with diagonal mass matrix are presented and their applicability in explicit dynamics is analyzed.

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Title: Heterogeneous Asynchronous Time Integrator for Impact and Contact Dynamics

Author(s): Fatima-Ezzahra Fekak, *Université de Lyon, INSA-Lyon* ; Michael Brun, *Anthony Gravouil, *Université de Lyon, INSA-Lyon*; Bruno Depale, *CETIM* .

During an earthquake, a bridge crane, usually located overhead in buildings, may be subjected to multiple impacts between crane wheels and rail. These multiple impacts cause significant damages in the structure which may fall on some critical structures in the building. Then the qualification of these structures with respect to normative seismic design requirements, which are continuously developing and becoming more and more stringent, requires strengthened simulation techniques especially to model the impact phenomenon. This thesis led by Cetim and LaMCos is aimed at more accurate modelling of the behavior of a bridge crane subjected to multiple impacts at an acceptable computational cost. The first part of our research work has led to the development of a new Lagrange explicit event-capturing contact/impact algorithm. The main advantages of this scheme are that no detection of events (impact or contact) is needed, no iterations are used to resolve the contact constraints and no additional numerical parameters are to be chosen by the user. The algorithm has an outstanding energy performance but need a refinement of the mesh in the contact area. This can be time-consuming while computing industrial structure like bridge cranes. A heterogeneous asynchronous time integrator is proposed. It allows to adopt the new explicit contact algorithm with the adequate mesh in the contact area and an implicit scheme with a coarse mesh in the rest of the domain. This method, developed by Gravouil and Combescure, is tested on an industrial contact/impact example. It gives accurate numerical results and a good energy performance at an acceptable computational cost.

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Title: An Inverse Finite Element Approach to Obtain Strain Rate Dependent Material Properties of the Human Intervertebral Disc

Author(s): Nicolas Newell, *Grigoris Grigoradis, Alexandros Christou, Diagarajen Carpanen, Spyros Masouros, *Imperial College London, UK*; J Paige Little, *Queensland University of Technology, Australia*.

Finite element (FE) models have been used widely to study injury biomechanics of the spine, however their precision depends upon accurate material properties, particularly of the intervertebral disc (IVD). Traditionally, these are obtained experimentally by excising tissue and loading it in tension and confined compression, or through indentation tests that can lead to inaccurate results as the disruption of the material continuity can affect its structural behaviour. To counter this, inverse FE modelling has been used, whereby properties of constituent components can be characterised without disrupting surrounding tissues. The aim of this study was to obtain strain-rate dependent material properties of the most influential components of the IVD in axial compression using inverse FE. For this initial investigation the vertebral bodies (VBs) of a human L3-L4 motion segment were sectioned transversely, and posterior elements and surrounding soft tissue was removed. 5mm of the VBs were fixed with bone cement in mounting cups with the transverse plane of the IVD aligned parallel to the workbench. After precycling, the specimen was axially compressed at 0.001, 0.01, and 0.1/s up to 15% strain. Specimens were allowed 5 minutes of relaxation between tests. The geometry for the FE model was obtained using custom developed image-processing software. Manually selected landmarks were imported into a pre-processing tool which generates the IVD mesh. Initial material properties were based upon existing literature values. The anulus ground matrix was modelled as a non-linear elastic material with 14 layers of embedded rebar elements to represent collagen-fibre bundles. The nucleus was modelled as an incompressible fluid with an initial pressure of 70 kPa. The lower VB was fixed and the upper VB was displaced at the same rate, and by the same amount as in the experiment. Experimentally, the IVD exhibited a non-linearly elastic behaviour, and stiffened with strain rate. A sensitivity study showed that the anulus ground matrix and fibre bundle material properties strongly influence the response, and were therefore obtained using an inverse FE optimisation algorithm. Optimised values of the modulus of the anulus fibre bundles ranged from 168 to 239 MPa, increasing with strain rate. The C10 value of the Mooney-Rivlin model for the anulus matrix increased with strain rate (range 0.001-0.039 MPa), while the C01 value decreased with strain rate (range 0.021-0.001 MPa). This technique can now be used on multiple specimens to determine average material properties of the IVD at a range of strain rates.

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Title: Foot and Ankle Injuries in Under-Vehicle Explosions: A Finite Element Study

Author(s): *Grigoris Grigoriadis, Diagarajen Carpanen, Anthony Bull, Spyros Masouros, *Imperial College London*.

In warfare incidents of anti-vehicular attacks, the most prevalent region of injury of the survivors has been the foot and ankle. Means for understanding the incident, assessing injury, and designing new mitigation strategies are invaluable in improving the injurious outcome. The use of validated computational models for the above purposes is a cost-efficient and repeatable alternative to labour intensive and expensive experiments. Since previous attempts are limited, the aim of this study was to develop, validate, and use a finite element (FE) model of the foot and ankle able to simulate under-vehicle explosions. The subject-specific FE model of the foot and ankle used in this study, was developed from MRI and CT scans of a cadaveric lower limb (male, 48 y.o.) using Mimics (Materialise HQ, Belgium) and MSC Marc (MSC.Software, USA). Cortical and trabecular bone, cartilage, and the plantar soft tissues were represented by tetrahedral elements. The forefoot was modelled as a single, rigid geometry and tension-only springs were used for the ligaments. Linearly elastic material properties were assigned to bone and cartilage while the plantar soft tissues were represented by a non-linearly viscoelastic material. The calf muscles mass was uniformly distributed around the long bones as point masses. The replicated loading conditions corresponded to different loading rates from experiments performed in three different traumatic injury simulators [1-3]. The comparison between computational and numerical responses for all different load-cases verified the ability of the model to simulate axial loading scenarios of different rates. Peak stresses were located on the medial side of the calcaneus and the distal tibia which are possible sites for fracture initiation. With increasing loading rates, the difference between peak axial force of the distal and proximal tibia was increased by 14% suggesting that the location of tibial fractures depends on the loading rate. The response of the model has been verified against data from a wide range of experimental conditions and the load pathway through the foot and ankle has been analysed. The model can now be used to assess the efficacy of existing and new mitigation strategies. References: [1] Crandall, 1996. Biomechanical response and physical properties of the leg, foot, and ankle. SAE 962424 Technical Paper. [2] Gallenberger et al., 2013. Biomechanics of foot/ankle trauma with variable energy impacts. Ann. Adv. Automot. Med. Annu. Sci. Conf. Assoc. 57,123–132. [3] Henderson et al., 2013. Biomechanical response of the lower leg under high rate loading. IRCOBI.

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Title: Designing Robust Beam Combinable High-Power Fiber Amplifiers

Author(s): *Jacob Grosek, *Air Force Research Laboratory*.

Beam combining is understood to be the most feasible path forward to achieving unprecedented power levels out of fiber laser systems. However, efficient beam combining architectures rely on having highly coherent light from each laser source. In order to reduce complexity and preserve system stability, it is important to extract as much power from each laser source as possible. Spatial and temporal coherency is difficult to maintain in high-power operation due to the deleterious repercussions of optical nonlinearities and thermal effects that arise in fiber amplifiers. The physics of electric fields propagating in microstructure fiber amplifiers can be studied through the use of finite element methods in order to optimize fiber designs such that they mitigate the detrimental effects that emerge in high-power operation.

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Title: Fluctuating Hydrodynamic Approaches for Fluid-Structure Interactions Subject to Thermal Fluctuations: Applications in Soft Materials and Fluidics

Author(s): Paul Atzberger, *Ben Gross, *University of California Santa*.

Fluctuating hydrodynamic descriptions provide a promising approach for meooscale modelling and simulation. We discuss methods and results for applications including the rheological responses of polymeric fluids, hydrodynamic coupling in lipid bilayer membranes, and transport within fluidic devices. We show how thermal fluctuations can be incorporated into models of fluid-structure interactions by building on the classical work of Landau-Lifschitz on fluctuating hydrodynamics. Using similar approaches from statistical mechanics, we develop Stochastic Immersed Boundary Methods and generalizations referred to as Stochastic Eulerian Lagrangian Methods. We show how these continuum descriptions can be effectively discretized using Finite Volume and Finite Element Methods for domains with complex geometries and how Ito calculus can be used to develop efficient time-step integrators for the stiff stochastic dynamics that arise in these systems. We then discuss results using these methods in various application areas including polymeric materials, lipid bilayer membranes, and fluidic devices. We then discuss our open source package MANGO-SELM for fluctuating hydrodynamic simulations available at http://mango-selm.org/.

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Title: A RB-VMS Modeling Framework for Sediment Transport: The Coupling of Turbulence and Rheological Behavior

Author(s): *Gabriel M. Guerra, *COPPE/UFRJ*; Souleymane Zio, Renato Elias, Fernando A. Rochinha, *Federal University of Rio de Janeiro*; Paulo Paraizo, *Petrobras*; Alvaro L.G.A. Coutinho, *Federal University of Rio de Janeiro* .

Turbidity currents are particle-laden flows that are a very complex natural phenomenon. Generally speaking, they are turbulent driven flows generated by fluids density difference that might be promoted by the presence of mixtures carrying sediments. They also are an important mechanism responsible for the deposition of sediments on the seabed. A detailed understanding of this phenomenon may offer new insight to help geologists to understand reservoir formation, a strategic knowledge in oil exploration. In this sense, numerical models can help to push forward the knowledge about complex dynamic physical systems. The modern approach to doing that involves detailed mathematical models. We present a finite element residual-based variational multiscale formulation applied to the numerical simulation of particle-laden flows in a Eulerian-Eulerian framework. Thus, the mathematical model results from the incompressible Navier-Stokes equation combined with an advection-diffusion transport equation. When sediment concentration is high enough, rheological empirical laws close the model, describing how sediment concentration influences the mixture viscosity. The present study represents an effort to quantitatively evaluate the effects of rheology on the dynamics of the flow like changes in the flow structures (turbulence) due to the presence of sediments or the resulting geometry of the basin deposits. With this aim, we use two scenarios for numerical experiments. The first is a lock-exchange configuration in a tank and the second employs a channel with a sustained current. Complex laboratory tests inspire both numerical experiments. We show how an empirical rheological law affects turbulent structures and quantities of interest, such as sediment deposition.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Hybrid CPU/GPU Parallel Unstructured Mesh Adaptation

Author(s): William Bussière, *François Guibault, *Ecole Polytechnique Montréal*.

This paper presents a novel parallelization approach to accelerate a tridimensional unstructured mesh adaptation algorithm controlled by a Riemannian metric. The proposed approach combines geometric adaptation operators implemented on a graphics processing unit (GPU) and topological operators implemented on CPU. Several geometric adaptation operators are compared, including Quality Laplacian [1], Nelder-Mead [2] and the Gradient Descent method, both in terms of performance and resulting mesh quality. Special attention is also given to the representation on GPU of the Riemannian control metric and its sampling during the adaptation process. A texture-based representation of the metric is adopted and the impact of metric resolution on mesh quality is studied. Overall, results indicate that similar final mesh quality may be obtained using the proposed accelerated adaptation approach when compared to the CPU-only version of the algorithm, with a ten-fold gain in performance over the parallel CPU-only version. [1] S. Lo, “Optimization of tetrahedral meshes based on element shape measures”, Computers & structures, vol. 63, no. 5, pp. 951–961, 1997. [2] S. Singer et J. Nelder, “Nelder-mead algorithm”, Scholarpedia, vol. 4, no. 7, p. 2928, 2009. DOI : 10.4249/scholarpedia.2928.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Construction and Identification of Stochastic Constitutive Laws for Soft Biological Tissues

Author(s): Brian Staber, *Université Paris-Est*; *Johann Guilleminot, *Duke University (CEE)*.

In this work, we address the construction, calibration and validation of stochastic hyperelastic constitutive laws for soft biological tissues. Towards this end, we first consider isotropic Ogden-type stored energy functions, and a stochastic model is constructed within the framework of Information Theory. Fundamental mathematical assumptions are specifically taken into account so that the stochastic stored energy function is almost surely consistent with existence theorems in nonlinear elasticity. An identification procedure is then proposed and applied by considering three experimental databases at various strain rates. It is shown that the stochastic model is able to accurately reproduce the experimental results (both in terms of mean behavior and variability), regardless of the tissue under consideration.

14th U.S. National Congress on Computational Mechanics
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Title: Adaptive Variational Multiscale Method for Turbulent Flows Past Complex Geometries

Author(s): *Ghalia Guiza, Mehdi Khalloufi, Philippe Meliga, Youssef Mesri, Elie Hachem, *Mines ParisTech - CFL*.

The use of adaptive methods to accurately predict aerodynamic coefficients or flow features is not a new practice, but is still a challenging topic where numerous questions remain unanswered. One such challenge concerns the anisotropic behavior for fully turbulent flows. It is also well known that when highly stretched elements are used, most of the classical numerical schemes tend to fail. We propose in this work a high order variational multiscale method to remedy this, with an adequate choice for the stabilization parameters. A new anisotropic mesh adaptation method had been implemented to deal with boundary layers and flow detachments in fluid structure interaction simulations with complex geometries [1,2]. The advantage of this method is its capability to deal with a multi-criteria adaptation such as the boundary layers, the velocity field and the turbulent eddy viscosity. Computational results are compared to existing data from the literature and to new experimental data from two industrial applications with complex geometries: a civil drone and a stratospheric airship. [1] L. Billon, Y. Mesri, E. Hachem, Anisotropic boundary layer mesh generation for immersed complex geometries, Engineering with Computers, pp. 1-12, 2016 [2] Y. Mesri, M. Khalloufi, E. Hachem, On optimal simplicial 3D meshes for minimizing the Hessian-based errors, Applied Numerical Mathematics, Vol. 109, pp. 235-249, 2016

14th U.S. National Congress on Computational Mechanics
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Title: Failed Rib Regions in a Computational Human Model vs. Observed PMHS Fractures: A Comparative Study

Author(s): *Berkan Guleyupoglu, Ryan Barnard, Scott Gayzik, *Wake Forest School of Medicine*.

Road traffic injuries are a large and growing share of the global health burden. The thorax is the second most commonly-injured body region in such incidents. ATDs are commonly used to determine thoracic injury risk based on correlative predictions; however localized injury is beyond their current capability. Rib strains can be measured on PMHS, but overhead requirements and specimen variability complicates their use. Computational human body models provide another potential avenue for study and have been used in kinematic and kinetic studies. However, development of robust localized injury criteria requires further comparison of model outcome to experimental injury. The objective of this study is to compare rib failed regions (FRs) from a computational human body model using two different methods vs. PMHS rib fractures observed in published tests. The GHBMC 50th percentile male occupant model (M50-O, v4.3) was used in all simulations. Fourteen simulations were conducted with rib FRs predicted probabilistically (PFR) or deterministically (DFR). The impacts were as follows: 6.7 m/s chest, shoulder, and thoracoabdominal hub, 12.0 m/s lateral plate, 6.0 m/s abdominal bar, 10 m/s lateral pelvic block, and 6.7 m/s Heidelberg-type lateral sled. Prediction of DFRs required analysis of eliminated elements, based on effective plastic strain exceeding 0.018 in 4 contiguous elements. Prediction of PFRs utilizes maximum principle strains in the ribs and assumes an age of 35 years. In the pelvic block impact there was 1 DFR and 2 PFRs compared with an average of 1.5 fractures found experimentally. The lateral plate impact had higher predictions with 43 DFRs and 28 PFRs whereas the average in the study was 22.5 fractures. The PMHS chest hub impacts had 9.4 ± 7.2 fractures and in our simulations, 5 DFRs and 11 PFRs were predicted. Finally, in the lateral sled case, 21 PFRs and 26 DFR's were predicted compared to an average of 14 fractures. The average age of PMHS was 64.8 years. The criteria for FRs should to be further tuned to match experimental values. When fracture counts are high experimentally, both FR predictions surprisingly exceed it despite the lack of eliminated elements in the PFR scheme. However, in cases where fractures were low, better agreement was found between experimental, FR predictions. Future work will focus on the effect of cortical thickness, and age as a predictor; either making material adjustments as function of age in the DFR scheme or explicitly in the PFR scheme.

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Title: Self-Supporting Structure Design in Additive Manufacturing through Moving Morphable Component/Void (MMC/MMV) Based Explicit Topology Optimization

Author(s): *Xu Guo, Weisheng Zhang, *Dalian University of Technolog*.

One of the challenging issues in additive manufacturing (AM) oriented topology optimization is how to design structures that are self-supportive in a manufacture process without introducing additional supporting materials. In the present contribution, it is intended to resolve this problem under an explicit topology optimization framework where optimal structural topology can be found by optimizing a set of explicit geometry parameters. Two solution approaches established based on the Moving Morphable Components (MMC) and Moving Morphable Voids (MMV) frameworks, respectively, are proposed and some theoretical issues associated with AM oriented topology optimization are also analyzed. Numerical examples show that the proposed approaches do have the capability to find optimized designs where overhang angle constraints can be fully respected. Besides optimal structural topology, the build orientation of AM can also be optimized with use of the proposed approaches in a straightforward way. Compared with existing approaches, the distinctive feature of the proposed approach is that it solves the corresponding problem through a totally explicit treatment. Furthermore, extending the proposed methods to three dimensional (3D) problems can be achieved by introducing 3D printable features in the problem formulation.

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Title: Alternating Direction Isogeometric L2 Projections in Cloud Environment

Author(s): *Grzegorz Gurgul, Marcin Los, Danuta Szeliga, Maciej Paszynski, *AGH Krakow, Poland*.

The idea of Alternating Direction Solver initially proposed by Victor Calo [1] can be a subject to massive parallelization as we proved in our work presented at 2016 IGA-MF conference held in La Jolla, California [2]. While this CUDA-based approach displays outstanding performance when compared to CPU-based implementations, it has some flaws. First, it can only scale up meaning that larger problems which cannot fit in the physical memory of the machine it runs on cannot be solved. Second, it has very limited portability being tied to a certain technology which is available only on certain hardware. Third, it is implemented at very low-level making it hard to introduce any changes and solve another problem in particular. This is why we decided to create a new implementation of Alternating Direction Solver, designed to run on In-Memory Data Grids such as Hazelcast clusters. This makes such solver scale out meaning that the maximum size of the problems solved and the minimum time to solve such problems are the function of the number of worker nodes used. We investigate this feature solving a series of large time-dependent problems from material science. In addition to this unbounded scalability we also focus on portability, testability and general feasibility. We achieve portability by using platform-independent Java language. We also ensured that the solver being primarily meant to be run in a cloud environment such as Amazon Web Services can also be run seamlessly in any local environment or virtualized Docker-based cloud-like environment. This feature and the fact that the Solver coding style conforms to object-oriented programming paradigm makes it easy to test and to understand. The solver can also be easily adjusted the to solve any other similar problem of any size and for any time step count. [1] L. Gao, V. M. Calo, Fast isogeometric solvers for explicit dynamics, Computer Methods in Applied Mechanics and Engineering 274, 19-41, 2014. [2] G. Gurgul, M. ■o■, A. K■usek, W. Dzwinel, M. Paszy■ski, Fast isogeometric L2 projections algorithm with GPU accelerators for modeling of tumor growth, 13th USACM thematic conference on isogeometric analysis and meshfree methods: Abstracts, 52, 2016 Acknowledgement: This work has been supported by Dean's grant from Faculty of Computer Science, Electronics and Telecommunications, AGH University, Krakow, Poland and by NCN, Poland grant no. 2015/19/B/ST8/01064.

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Title: A Partitioned Iterative Interface Force Correction Scheme for Fluid-Flexible Multibody Interaction

Author(s): Ritwik Ghoshal, *Research Fellow, NUS*; *Pardha Gurugubelli, *Research Engineer, NUS*; Anurag Yenduri, *Engineering Analyst, Oceaneering*; Rajeev Jaiman, *Assistant Professor, NUS*.

A novel partitioned iterative interface force correction scheme is developed to simulate strong fluid-structure-interaction (FSI) due to flow-induced vibration of flexible multibody system (viz., offshore floating platforms coupled with production risers and station keeping system) in aturbulent flow.The structural domain with multibody systemsis modeled via nonlinear corotational finite element method,whereas the fluid domain is solved using the Petrov-Galerkin finiteelement method for moving boundary Navier-Stokes solutions.Turbulence effects are modeled explicitly via delayed detached eddy simulation (DDES) and discretized through the recently developed positivity preserving variational (PPV) scheme. The temporal discretization for the fluid equation is embedded in the generalized-α framework by making use of theclassical Newmark approximations in time. However, for the solid domain, a time discontinuous Galerkin method based on energy decay inequality is utilized, since it is proven to be stable and accurate for flexible multibody systems with constraints. The proposed partitioned iterative scheme relies on the combinedinterface boundary conditions and non-linear interface force corrections for numerical stabilization of the variational coupledsystem based on the Navier-Stokes and flexible multibody equations with constraints. The incremental velocity and pressure are computed withmatrix-free implementation of the restarted Generalized Minimal RESidual (GMRES) solver which uses a diagonal preconditioner and a Krylov space of orthonormal vectors. Newton-Raphson type iterations are utilized to minimize the linearization errors per time step and satisfy the equilibrium of forces along the fluid-flexible multibody interface. A systematic comparative study of the coupling is performed using classical problems of flow-induced vibration used for benchmark. An application of the partitioned iterative interface force correction scheme for fluid-flexible multibody interaction is demonstrated by simulating the flow induced vibration of an offshore platformconnected to production and station keeping systems submerged in a fluid domainmodeled with the Navier-Stoke equation.

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Title: Crash Analysis and Evaluation of Vehicular Impacts on W-Beam Guardrails Placed behind Curbs Using Finite Element Simulations

Author(s): *Matthew Gutowski, Emre Palta, Howie Fang, *UNC Charlotte*.

Roadway design, including the use of traffic barriers, is a critical aspect in transportation safety and it reduces the severity and frequency of automotive accidents. All barriers used on U.S. highways are designed according to the American Association of State Highway and Transportation Officials (AASHTO) Roadside Design Guide and they are tested to ensure they satisfy the safety criteria specified by Manual for Assessing Safety Hardware (MASH). While a curb's main functions are to separate the road from roadside, control vehicle right-of-way, and channel water runoff; curbs are discouraged by AASHTO from being installed on high-speed roadways due to the obstructive nature caused when vehicles strike them. The destructive characteristics of vehicular crashes impose significant challenges to barrier design using full-scale vehicle testing; numerical simulations thus become a viable option to support guardrail design improvements and performance evaluation. In this study, validated vehicle models and W-beam guardrails installed behind AASHTO Type B curbs were used to perform full-scale simulations of vehicle-curb-guardrail impacts. Seven single-faced W-beam guardrails [1] (with placement heights of 27, 29, and 31 inches) placed behind curbs at zero, six, and twelve feet offsets were impacted at 44 mph (70 km/h) and two impact angles (15■ and 25■) by a small passenger car (1996 Dodge Neon) [2] and a large pickup truck (2006 Ford F-250) [3]. The guardrail's performance was evaluated by analyzing the vehicular responses based on post-impact exit trajectory utilizing the MASH exit-box criterion, rotational angles, and transverse displacements and velocities. [1] Opiela, K., Kan, S., Marzougui, D. Development of a Finite Element Model for W-beam Guardrails. Report NCAC 2007-T-004, National Crash Analysis Center (NCAC), George Washington University, Ashburn, VA; 2007. [2] Opiela, K., Kan, S., Marzougui, D. Development & Validation of a Finite Element Model for the 1996 Dodge Neon Passenger Sedan, Report NCAC 2007-T-007, National Crash Analysis Center (NCAC), George Washington University, Ashburn, VA; 2007. [3] Opiela, K., Kan, S., Marzougui, D. Development & Validation of a Finite Element Model for the 2006 Ford F250 Pickup Truck. Report NCAC 2008-T-003, National Crash Analysis Center (NCAC), George Washington University, Ashburn, VA; 2008.

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Title: A New Energy-Based Solder Joint Fatigue Life Prediction Approach for Electronic Packages

Author(s): Forrest Baber, *Ibrahim Guven, *Virginia Commonwealth Univ.*.

A novel methodology for predicting fatigue life in metals is presented. The underlying premise is that material degradation through energy dissipative mechanisms play a central role in crack initiation and propagation. The new method uses peridynamic approach in simulating crack initiation as well as propagation. Dissipated energy in the vicinity of newly generated surfaces such as fractures are calculated as the cracks propagate. The dissipated energy is subsequently correlated with the crack propagation rate. The most severe deformation state during a loading cycle is taken as the static loading applied to the peridynamic model. Assuming that fatigue cracks follow paths similar to cracks form under quasi-static loading, critical stretch material parameter of the peridynamic approach is gradually reduced to allow for the most deformed regions to fail first. Once failures start taking place, load rebalance leads to further propagation. By reducing the critical stretch gradually, it is ensured that the fracture is not dynamic in nature. The method is first demonstrated using controlled experimental measurements of compact tension test specimens that were subjected to mechanical loading only. The current approach predicts cracks paths with high accuracy. The fatigue life predicted by simulations of compact tension test specimens are within 12% of the measurements. The methodology is then applied to solder joint fatigue problems. The nonlinear thermo-mechanical problem is first solved by finite element analysis for four thermal cycles. The most severe deformation configuration during the fourth thermal cycle at the most critical solder joint is identified and applied as the static loading in the peridynamic simulation. Number of cycles to crack initiation and propagation on five distinct packages are predicted. The combined finite element and peridynamic approach yielded predictions within 25% of the experimentally measured fatigue life values for four packages. In the fifth package, a close match is not achieved. Overall, the results point to the conclusion that the peridynamic approach has great potential to accurately predict solder joint fatigue life.

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Title: IMPETUS – Interactive MultiPhysics Environment for Unified Simulations

Author(s): *Vi Ha, George Lykotrafitis, *University of Connecticut, USA*.

We introduce IMPETUS – Interactive MultiPhysics Environment for Unified Simulations (Ha and Lykotrafitis 2016), an object-oriented, easy-to-use, high performance, C++ program for three-dimensional simulations of complex physical systems. The program uses Message Passing Interface (MPI) for parallel computing operations and utilizes contemporary object-oriented programming techniques to provide an interactive and easily customizable coding environment for users to develop complex multi-physics simulations. There is currently no generally accepted High-Performance Computing software available that inherently incorporate interactions and communication between particles and between particles and their environment. To solve this problem, we introduce a simulation environment that incorporates three cross-interacting domains named Modular Interactive Domains (MIDs): spatial short-range particle dynamics domain, long-range network domain, and interactive continuum field domain. Short-range particle dynamics domain uses spatial distribution to allocates particles to processors according to their positions to attain high efficient short-range MD computations. The global long-range network domain allows efficient interaction between particles regardless of their spatial position or the processors they reside within the computing cluster. The third interaction domain is the continuum space domain which employs an explicit finite difference algorithm to solve the parabolic equation. The continuum domain allows communication between particles or between particles and the environment via diffusion. All three MIDs can interact with each other and are efficiently parallelized via MPI; they can run simultaneously in the same simulation. All simulations and models are created using different combinations and different numbers of MIDs. The concept of utilizing MID classes and subclasses reduces development time, ensures accuracies and greatly diminishes human errors. IMPETUS can be employed in numerous biological cases and benefit a large variety of research areas. For example, calculations of the chemotactic response of cells moving in the spatial domain and subjected to a chemical concentration gradient in the continuum domain are perfectly feasible. Users can also easily simulate more complex scenarios such as a coarse-grained models of diffusion of cell membrane proteins on a lipid bilayer. Another example is a simulation of a mixture of molecules of different sizes and properties by creating several MIDs with different cut-off radius to avoid impairment of computational efficiency. Reference Ha, V. Q. and G. Lykotrafitis (2016). "IMPETUS – Interactive MultiPhysics Environment for Unified Simulations." Journal of Biomechanics 49(16): 4034-4038.

14th U.S. National Congress on Computational Mechanics
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Title: Barrier-Free Parallel–Adaptive Scheme for Asynchronous Spacetime Discontinuous Galerkin Methods

Author(s): *Robert Haber, *University of Illinois at Urbana-Champaignna-Champaign*; Amit Madhukar, Volodymyr Kindratenko, *University of Illinois at Urbana-Champaign*; Reza Abedi, *University of Tennessee Space Institute (UTSI) / Knoxville (UTK)*.

This presentation describes a new architecture for parallel–adaptive simulation using asynchronous Spacetime Discontinuous Galerkin (aSDG) methods. The new architecture abandons two mainstays of conventional parallel finite element computation: the bulk synchronous parallel (BSP) model and the Domain Decomposition Method (DDM). The BSP model is naturally incompatible with the aSDG method and is also emerging as an obstacle to achieving exascale computing goals. Therefore, we opt for a barrier-free asynchronous design. In previous work, we obtained near-perfect scaling with static domain decompositions and non-adaptive aSDG models using Charm++, but we found that revising the domain decomposition for load balancing was too cumbersome and far too slow to keep up with the fine granularity of aSDG adaptive meshing. Our solution was to parallelize the fundamental aSDG operations — spacetime patch construction, local finite element solution, and adaptive remeshing — at their common granularity: a single patch. In the case of adaptive meshing, this requires a modified algorithm called lazy refinement. In view of the uniform locality of the resulting aSDG algorithm, the advantages of domain decomposition into contiguous subdomains vanish. Load balance is controlled by the assignments of vertices in the space-like front mesh to the available cores, as these assignments determine where spacetime patches are handled. Rebalancing the load reduces to modifying the per-vertex pointers that determine these assignments, a simple, lightweight procedure that is executed at the same patch-level granularity as the rest of the algorithm. We present results from strong scaling studies to demonstrate the effectiveness of this new parallel architecture.

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Title: A Rate-Dependent Interfacial Damage Model for Multiscale Dynamic Fracture

Author(s): Reza Abedi, *University of Tennessee Space Institute*; *Robert Haber, *University of Illinois at Urbana-Champaign*.

Dynamic fracture in brittle and quasi-brittle materials is a multi-scale, multi-physics problem, with rapidly evolving geometry and complex failure mechanisms triggered by microscopic flaws. This presentation describes a new interfacial damage model for dynamic fracture and its application within an adaptive, asynchronous Spacetime Discontinuous Galerkin (aSDG) model for high-resolution multi-scale fracture simulations. We use a novel interfacial damage model to represent the fracture process. Rather than use damage to degrade an interfacial stiffness or traction-separation law, we use a scalar damage parameter to interpolate between bonded and debonded Riemann solutions, consistent with the governing equations in the bulk material. The Riemann solutions for debonded conditions account for separation, contact–stick and contact–slip modes, so crack opening, closure, and slip are handled in a dynamically consistent fashion. We introduce a new two-term damage evolution rule in which the traction acting across a potential fracture surface initiates and drives early stages of the damage evolution, while the velocity jump across the interface (i.e., opening and slip velocities) drives the later evolution. This provides more realistic response because the velocity term allows allows damage accumulation to continue, even if tractions fall below their critical threshold, as is consistent with the inertial aspects of dynamic fracture. Nucleation of new cracks is governed by a probabilistic description of microscopic flaws. Simulation examples demonstrate our model's ability to capture multi-scale fracture features, such as crack oscillations, micro-cracking and crack branching as well as the influence of loading and the stochastic microscale flaw model on the crack-pattern morphology.

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Title: Adaptive Variational Multiscale Method for Non-Newtonian Multiphase Flows

Author(s): *Elie hachem, Stephanie Riber, Youssef Mesri, Rudy Valette, *Mines ParisTech - CFL*.

The simulation of Non-Newtonian flows is still attracting considerable attention in many industrial applications. However, the underlying numerical discretization and regularization may suffer from numerical oscillations, in particular for low inertial number, or high Bingham [1] and Reynolds numbers flows. In this work, we investigate the Variational Multiscale stabilized finite element method in solving such flows. We extend it for the first time to two-phase flows using a volume preserving Levelset method [2,3]. Combined it with a posteriori error estimator for anisotropic mesh adaptation, it enhances considerably the use of regularization. Computational results, including new results on continuum granular flow, are compared to existing data from the literature or to experimental data from industrial applications. [1] S. Riber, Y. Mesri, R. Valette, E. Hachem, Adaptive Variational MultiScale Method for Bingham flows,Computers & Fluids, Vol. 138, pp. 51-60, 2016 [2] E. Hachem, M. Khalloufi, J. Bruchon, R. Valette, Y. Mesri, Unified adaptive Variational MultiScale method for two phase compressible-incompressible flows, Computer Methods in Applied Mechanics and Engineering, Vol. 308, pp. 238-255, 2016 [3] M. Khalloufi, Y. Mesri, R. Valette, E. Hachem, High fidelity anisotropic adaptive variational multiscale method for multiphase flows with surface tension, Computer Methods in Applied Mechanics and Engineering, Vol. 307, pp.44-67, 2016

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Title: Adaptive Cross Approximation in BEM for Elastic Continua

Author(s): *Anita Maria Haider, Martin Schanz, *Graz University of Technology*.

The study of deformation of elastic bodies is of interest in many fields of engineering. Typical problems related to such media are wave propagation phenomena. Further research, driven by industrial applications, is dedicated towards studying elastic deformations due to thermal loads. Such problems can be treated by the boundary element method in an elegant manner. However, the classical boundary element method leads to fully populated matrices. This approach is prohibitive due to its excessive requirements of memory and computing time. To overcome these drawbacks we carry out a low rank approximation by means of the adaptive cross approximation. One crucial step of this algorithm is to find a suitable pivot element. While this is straightforward for scalar-valued problems, it poses some difficulties for vector-valued problems, like elastodynamics or thermoelasticity. This talk is devoted to the approximation of boundary element matrices via adaptive cross approximation. First, a model problem of linear elasticity is introduced. Equivalent representations of its solution using boundary integral equations are discussed. Once the discretization of these equations is established, we focus on the approximation of the occurring matrices. We recall the principles of the adaptive cross approximation and address the search of a suitable pivot element. Finally, the results of numerical experiments are presented and discussed. They show that the boundary element matrices can indeed be compressed significantly while retaining a good quality of the solution of the underlying problem. Moreover, a substantial reduction of the computation time is observed.

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Title: Eigenlocking in Shells of Revolution

Author(s): *Harri Hakula, *Aalto University*.

The finite element modeling of shells is known to be a very demanding task because of the many different ways parametric error amplification or locking phenomena can occur. Here we consider locking in connection with eigenvalue problems in shells, especially in inhibited pure bending shells or shells with clamped support. Our purpose is not to suggest ways for alleviating or circumventing eigenlocking, but to analyse, predict, and demonstrate its existence when the lowest eigenfrequency is computed. The concept of locking in parabolic shells was first identified in [1], but never fully demonstrated through numerical experiments. The results obtained for hyperbolic shells are new and the main contribution of this talk. As a by-product of our analysis, we also solve the so-called ”hyperbolic packing problem” concerning the relation of the angular and axial wave numbers of the lowest eigenmodes of hyperbolic shells. References: [1] L. Beirao da Veiga, H. Hakula and J. Pitkäranta. Asymptotic and numerical analysis of the eigenvalue problem for a clamped cylindrical shell, M3AS, 18, 11(2008), 1983-2002.

14th U.S. National Congress on Computational Mechanics
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Title: Two Finite Element Solvers and Mesh Techniques to Evaluate Lower Leg Protections

Author(s): *Carolyn Hampton, Michael Kleinberger, *Army Research Laboratory APG*.

Developing a finite element human body model is challenging but necessary to computationally evaluate protective equipment for vehicle occupants. In this study a finite element model of the lower leg was developed for biomechanical evaluation of footwear for blast and blunt impacts. Methodology: Two finite element codes, LS-DYNA and ParaDyn, were used to simulate seven 3.4 – 5.8 kg, 5 – 10 m/s axial pendulum impact experiments [1] into unprotected lower legs producing above-tibia forces of 3.2 – 12.1 kN. All legs were ballasted to 11.5 kg. Material properties for trabecular and cortical bone and soft tissue [2] were collected from literature. Hexahedral and tetrahedral finite element meshes were generated from a CT scan of a healthy young adult male. Simulations were evaluated by comparing force-time and peak force against experiments. The force response sensitivity to the soft tissue material parameters (density, collagen fiber strength, matrix strength, viscosity, and bulk modulus), mass distribution, and friction were evaluated. The foot arch height and explicitly represented foot ligaments were evaluated by modifying the original mesh. Results: The pendulum impact simulations produced forces of 3.6 – 12.7 kN and captured the post-impact tensile phase up to 1 kN. The ParaDyn peak forces were -1.6% compared to LS-DYNA with nearly identical force-time curves. A finite element boot was added and was found to reduce peak force by 33% for a 5 m/s impact compared to 40% experimentally. Peak forces from the hexahedral leg were softer compared to the tetrahedral leg and was partially addressed with improved soft tissue fiber characterization [3]. The soft tissue fiber response dominates that of the matrix. Eliminating viscosity reduced peak force (17%) and increased duration (1.9 ms). Similar, subtler effects were observed with the bulk modulus. Increased mass distribution into the soft tissue reduced impact severity. Flattened arches and strengthened foot ligaments increased peak forces. Conclusions: LS-DYNA and ParaDyn simulation force results were equivalent, but the results were influenced by several parameters that naturally exhibit wide variability. The force responses matched well both with and without a boot, demonstrating that finite element analysis can be used to evaluate protective equipment. Continued research will address other loading conditions, individual variations, posturing effects, and tradeoffs between tetrahedral and hexahedral meshes. References: [1] Gallenberger et al 2013 Annals Adv Auto Med 57. [2] Puso & Weiss 1998 J Biomed Eng 120(1). [3] Groves et al 2013 J Mech Behavior Biomed Mat 18.

14th U.S. National Congress on Computational Mechanics
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Title: Lineal-Path Function for Describing Pore Microstructures of Cement Paste and Relations to Mechanical Properties

Author(s): *Tong-Seok Han, Ji-Su Kim, *Yonsei University*.

Pore distribution of a cement paste strongly affects the mechanical behavior such as stiffness and strength. Porosity is the first order parameter which can be used to identify the complex pore microstructures of cement paste, but it has limitations as a scalar parameter. In this study, the lineal-path function [1], one of the low-order probability functions, of cement paste microstructures is investigated as a supplement or an alternative parameter for describing microstructural characteristics. In particular, the area of lineal-path function is used as a measure of pore microstructure characteristics which can be used to link with its properties. The phase field fracture [2] is used to evaluate the stiffness and tensile strength of cement paste microstructures and the evaluated properties are linked to the proposed characterization parameters. The evaluation is performed on virtual specimens obtained from micro-level computerized tomography images of real cement paste specimens. The validity of the microstructure-property relations obtained from the proposed characterization parameters and the crack phase field model are confirmed through the statistical analysis of dozens of specimens. It is concluded that the area of the lineal-path function shows very strong correlation with the mechanical properties. The parameter can be used as supplementary or even an alternative parameter to describe the pore microstructures of cement paste. In particular, the area of lineal-path function is used as a measure of pore microstructure characteristics which can be used to link with its properties. [1] B. Lu, S. Torquato, Lineal-path function for random heterogeneous materials, Phys. Rev. A 45 (1992) 922–929. [2] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Comput. Meth. Appl. Mech. Eng. 199 (2010) 2765–2778.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Improved Thermo-Mechanical Analysis of Laminated Composite Structures Using the New Enhanced First-Order Shear Deformation Theory

Author(s): *Jang-Woo Han, Maenghyo Cho, *Seoul National University*; Jun-Sik Kim, *Kumoh National Institute of Technology*.

With the increasing usage of advanced composite materials in high-temperature environments, the thermo-mechanical analysis of laminated composite structures becomes an important issue. This paper proposes a new type of conventional first-order shear deformation theory (FSDT) in order to accurately and efficiently analyze the thermo-mechanical behavior of laminated composite structures. The main objective herein is to systematically establish the relationship between the two independently assumed fields (displacement and transverse stress fields) via the mixed variational theorem. To this end, the transverse shear stress field is defined by the third-order zigzag model to improve the performance, whereas the displacement field is obtained from the conventional FSDT to amplify the benefits of the numerical efficiency. In the thermal loading problem, a profound consideration on the transverse normal strain effect is necessary for a reliable analysis. In order to take this effect into account, the transverse displacement field is assumed to be a smooth parabolic distribution by superimposing a prescribed thermal field. This allows one to consider the thermal transverse normal strain effect without introducing any additional unknown variables. The resulting strain energy expressions are collectively referred to as the enhanced first-order shear deformation theory including the transverse normal effect based on the mixed variational theorem (EFSDTM_TN). The proposed theory has the same computational advantages as the conventional FSDT. Further, the accuracy of the local solutions can be improved via a recovery procedure. In this procedure, in-plane correction factors are introduced and determined by applying equivalent stress resultants so that the improved stresses satisfy the plate equilibrium. Finally, the performance of the proposed theory are demonstrated by comparison of its results with exact solution as well as the results of other theories available in the literature. References [1] M. Cho, R.R. Parmerter, An efficient higher order plate theory for laminated composites, Compos Struct, 1992, pp. 113-123. [2] J.S. Kim, M. Cho, Enhanced modelling of laminated and sandwich plates via strain energy transformation, Compos Sci Technol, 2006, pp. 1575-1587.

14th U.S. National Congress on Computational Mechanics
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Title: Embedded Boundary Conditions for Plate Bending Problems

Author(s): *Isaac Harari, *Tel Aviv University*.

An efficient procedure for embedding kinematic boundary conditions in various plate bending models is based on a stabilized variational formulation, obtained by Nitsche's approach for enforcing surface constraints. Work-conjugate pairs weakly enforce kinematic boundary conditions. For thin plate problems, the absence of kinematic admissibility constraints allows the use of non-conforming meshes with non-interpolatory approximations, thereby providing added flexibility in addressing higher continuity requirements. The use of a scaling factor, induced by the plate thickness, leads to a formulation with a single stabilization parameter. The enforcement of tangential derivatives of deflections obviates the need for pointwise enforcement of corner forces in the presence of corners. The single stabilization parameter is determined from a local generalized eigenvalue problem, guaranteeing coercivity of the discrete bilinear form. The accuracy of the approach is verified by representative computations with bicubic B-splines, providing guidance to the determination of the scaling and exhibiting optimal rates of convergence and robust performance with respect to values of the stabilization parameter. For shear-deformable plates, the absence of kinematic admissibility constraints facilitates the use of approaches that are insensitive to shear locking. Again, the use of the scaling factor, more closely linked to the plate thickness in this case, leads to a formulation with a single stabilization parameter, which is determined from a local generalized eigenvalue problem, guaranteeing coercivity of the discrete bilinear form. The accuracy of the approach for standard formulations of shear-deformable plates is verified by representative computations with bicubic B-splines, confirming the interpretation of the scaling and exhibiting optimal rates of convergence and robust performance.

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Title: Fracture of Nano-Particle Reinforced Polymers: Bridging the Scales from Micro to Macro

Author(s): *Ajay Bangalore Harish, Peter Wriggers, *LUH Hannover*.

Modeling of fracture in large deformation context has continued to remain a challenge in spite of the growth in mechanics. Fracture at the macroscale is significantly influenced by changes at the microscale. It is thus necessary to understand the changes at the micro scales and their relevance to macroscale fracture. In this work, scale-relevant models are used at the micro- and macro-scales to understand the effects of fracture phenomenon across the scales. Nonlocal cohesive zone models are used for scale transfer. While on one end of the spectrum, i.e. macroscopically, polymeric materials exhibit extensive influence of the mechanical properties on temperature and strain-rate. At low temperatures, they exhibit highly brittle behavior and with increasing temperature (especially across the glass- transition temperature) they demonstrate a brittle-to-ductile transition. While glassy polymers exhibit significant crazing, rubbery and nano-particle reinforced rubbery polymers demonstrate moderate crazing during fracture. The macroscopic fracture is accompanied by several microscopically-motivated effects like cluster breakage, Mullins and Payne effects. This work presents a thermodynamically consistent and physically motivated constitutive model at the microscale capable of accounting for clustering effects and alongside also several effects like the Mullins and Payne effects. This work only considers non-crystallizing filled elastomeric systems. Further on, the model accounts for breakage of clusters and debonding of polymers as cause of relative weakening of their interfaces and fracture of the overall microstructure. In this work, microscopic parameters that can influence the overall fracture process at the macroscale are identified and used as inputs to the nonlocal cohesive zone model. Hybrid nonlocal cohesive zone elements are used in the simulation of fracture phenomena at the and further on these simulations are further validated through nanoindenter scratch experiments. While concurrent multiscale models that can bridge between statistical mechanics and hyperelastic models would be an ideal scenario, such approaches are computationally infeasible today. The above proposed sequential multiscale models provide a more viable alternative to understand the origins of macroscopic fracture in nanoparticle-reinforced polymeric materials. References [1] A. B. Harish, P. Wriggers, “Mesoscale constitutive modeling of non-crystallizing filled elastomers,” Computational Mechanics, Vol. 57(4), pp.653-677 (2016) [2] J. Diani, B. Fayolle, and P. Gilormini, “A review on the Mullins effect,” European Polymer Journal, Vol. 45(3), pp.601-612 (2009) [3] J. Diani, M. Brieu, J.-M. Vacherand, and A. Rezgui, “Directional model for isotropic and anisotropic hyperelastic rubber-like materials,” Mechanics of Materials, Vol. 36(4), pp.313-321 (2004)

14th U.S. National Congress on Computational Mechanics
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Title: Adaptive Wavelet Algorithm for Solving Coupled Systems of Nonlinear Partial Differential Equations with Error Control

Author(s): *Cale Harnish, Karel Matouš, *University of Notre Dame*; Daniel Livescu, *Los Alamos National Laboratory*.

As the field of computational physics has matured, the engineering applications which we seek to model have grown remarkably in size and complexity. Modern simulations solve coupled systems of nonlinear partial differential equations (PDEs), with multiphysics features evolving on a wide range of spatial and temporal scales. In these situations, traditional numerical methods may impose prohibitive computational requirements by using a highly resolved uniform grid. We present a novel wavelet based algorithm developed to overcome the computational difficulty of these multiscale problems. Our proposed numerical method is a pseudo-spectral technique which exploits the features of the biorthogonal interpolating wavelet family of basis functions, and second generation wavelets, to solve initial-boundary value problems on finite domains. We maximize the data compression ability of these bases by creating a unique multiresolution representation for each unknown, and using the minimum number of collocation points to define the coarsest resolution. Moreover, we compute spatial derivatives by operating directly on the wavelet bases. We derive new error estimates for the wavelet representation of fields, their derivatives, and the aliasing errors associated with the nonlinear terms in a PDE. Then, our estimates are used to construct a sparse multiresolution spatial discretization that a priori guarantees the prescribed accuracy for each unknown. We have developed a predictor-corrector strategy within our time advancement procedure to dynamically adapt the computational grid and maintain the prescribed accuracy of the solution of the PDE as it evolves. Furthermore, we introduce a simple matrix notation for wavelet operations to facilitate the optimization of their computational implementation. Our highly adaptive method has been verified on a variety of nonlinear problems including Burgers' equation and the Navier-Stokes equations. Exponential convergence to the analytical solutions is achieved at a rate which is in agreement with a priori estimates. Our algorithm provides accurate solutions to coupled systems of nonlinear PDEs with explicit error control, significant data compression, and bounded global energy conservation.

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Title: Multiscale Thermodynamics: Toward a Precise Description of the Microstructural Evolution of Complex Materials

Author(s): *Jean-Philippe Harvey, Aimen Gheribi, *École Polytechnique Montréal*.

The judicious selection of materials used for specific technological applications is at the heart of most engineer's practices: chemical engineers will try to limit wear and corrosion of their high temperature reactors; civil engineers will design bridges that can tolerate specific loads and climate variations while mechanical engineers will select materials that ensure the highest theoretical efficiency of their energy conversion units that are turbines, motors, pumps, etc. In all these applications, a fundamental understanding of the impact on the thermo-physical properties of the initial microstructure of a material as well as its subsequent evolution in service are required. The initial microstructure of a material is directly linked to the thermo-mechanical history that led to its elaboration. The initial microstructure of a material might be in a metastable/unstable state such as metallic regions close to welds or for plastically deformed parts. At the opposite, a material could be in a highly stable initial state generated by controlled heat treatments frequently used for metallic alloys. In both cases, thermodynamics will define the driving force the potential microstructural evolution in service. The different constraints imposed by the environment to the studied system that are the temperature, the pressure, the chemical potential, the stress, the strain, etc. will define the theoretical final state that could be reached from thermodynamic considerations only. To quantify the microstructural evolution as a function of time, kinetics theories will ultimately need to be coupled to such thermodynamic calculations if a robust approach is to be implemented. In this work, we present the first step toward a precise description of the microstructural evolution of complex materials, i.e. the definition of the next generation of thermodynamic models that describe the energetic behavior of complex materials. In our new approach, we propose to explicitly define all the energetic contributions to the Gibbs free energy that are the internal energy, the purely mechanical PV work contribution, as well as the configurational and vibrational entropies. We present here an original approach to integrate atomistic theoretical models used to express the electrostatic forces at the origin of chemical bonds into statistical models that account for both the short range and long range chemical environment. This approach allows a fine description at the macroscopic level of the phase assemblage, a key ingredient required to define the microstructure of a material.

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Title: VMS A Posteriori Error Estimation for Stokes Flow

Author(s): *Guillermo Hauke, Diego Irisarri, *EINA*.

The genesis of stabilized methods was established in [1] from the standpoint of the variational multiscale theory (VMS). By splitting the solution into resolved and unresolved scales, it was shown that stabilized methods take into account an approximation of the unresolved scales into the finite element solution. Previous works have shown that these unresolved scales contain fairly accurate error information that can be exploited to formulate explicit a posteriori error estimators which are consistent with the assumptions inherent to stabilized methods [2]. The proposed technology, which is especially suited for fluid flow problems, is very economical and can be implemented in standard finite element codes. It has been shown that, in practice, the method is robust uniformly from the diffusive to the hyperbolic limit [2]. Lately, attention has been given to fast calculation of the pointwise error [3]. In this presentation new highlights will be given about a posteriori estimation of the global, local and pointwise error for Stokes flow. [1] T.J.R. Hughes, Multiscale phenomena: Green's functions, the Dirichlet-to-Neumann formu- lation, subgrid scale models, bubbles and the origins of stabilized methods. Comput. Meth. Appl. Mech. Engrg. 127, 387–401, (1995). [2] G. Hauke, D. Fuster and M.H. Doweidar, Variational Multiscale a-Posteriori Error Estimation for Multi-dimensional Transport Problems. Comput. Meth. Appl. Mech. Engrg. 197, 2701– 2718, (2008). [3] D. Irisarri, G. Hauke, A posteriori pointwise error computation for 2-D transport equations based on the variational multiscale method. Comput. Meth. Appl. Mech. Engrg. 311, 648–670, (2016).

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Title: A Plate Element Formulation for Modeling Progressive Damage and Failure of Shear Deformable Laminates

Author(s): *Devlin Hayduke, *Materials Sciences Corp.*.

Advanced composite material systems are vital to the development of lightweight, multi-functional aerospace structures. In addition to reducing the weight of the structure, these material systems provide the ability to expand the function of the structure by tailoring stiffness and strength characteristics for numerous applications. Consequently, carbon fiber-reinforced epoxy structures have become very attractive for airframe applications. It is normally accepted that a limiting characteristic of laminated composite structures of this nature is the response of the impacted material to compressive loads, such as buckling. It is also well documented that delamination is the predominant damage mode in composite materials subjected to impact damage. Novel advanced composite material design and analysis approaches are sought to minimize the risk of damage from low-energy impacts resulting from operations and maintenance impact accidents. An analysis tool that contains novel mathematical/physical approaches for accurately assessing the residual compressive strength in impact-damaged composite structures is desired. In response to this need, a user element (UEL) subroutine for use with commercially available analysis codes has been developed by Materials Sciences Corporation. In particular, an improved plate formulation element that offers advantages in both the economy and reliability of computations has been realized. This novel UEL formulation integrates a nonlinear material model to evaluate progressive damage and failure of composite materials on a ply-by-ply basis while incorporating a shear correction model that accurately predicts the nonlinear transverse response of impacted composite structures. A brief overview of the theoretical formulation of the element and embedded nonlinear material model will be provided. Followed by examples of standard characterization tests and the corresponding data reduction methodology required to determine model parameters for a commonly used intermediate modulus carbon fiber reinforced epoxy material system. In addition, an example of the residual strength predictions for a standard test specimen that exhibits progressive damage due to transverse shear will be reviewed. Finally, results of analysis models, e.g., dynamic and quasi-static, that were used to predict residual strength of an impacted laminated panel will be compared to experimental results.

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Title: The Quick Continuum Structural Topology Optimization Based on the Changes of Supporting Conditions

Author(s): *jianjun he, *CSUST*.

This paper focus on the fast topology optimization under the changes of the supporting condition. Its modal analysis are based on the pseudo random number initialized vectors with the Rayleigh-Ritz analysis, which is simple to implement and can be directly extended for structural dynamic topology optimization. The optimization algorithm are the QSIMP (Quick SIMP) method, which is proposed by us in the other literature. The numerical examples show that the proposed method is effective with small computational cost and high efficiency, which can greatly reduce computational cost without affecting the outcome of the optimization process, and the topology optimization results are consistent with the other results obtained by commonly used optimization methods, such as the SIMP-based optimization method or the GA-based optimization method, etc. Meanwhile, the introduction of approximate modal analysis based on the pseudo random number initialization leads to the certain randomness and sub-optimal multiplicity of topology optimization results, thus the proposed mixed optimization design method could enlarge the global search ability of the fundamental SIMP-based method to some extent.

14th U.S. National Congress on Computational Mechanics
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Title: Fractures with Constricted Opening

Author(s): *Junxian He, *University 0f WesternAustralia*; Elena Pasternak, Arcady Dyskin, *University of Western Australia*.

One of the forms of material instability and failure considered traditionally is the growth of Mode I fractures or cracks. Cracks in heterogeneous materials often contain bridges that are parts of unbroken material connecting the opposite faces of the fracture. Bridges are usually attributed to the fracture process zone. We show by direct experiments and observations that in rocks and concrete the bridges are distributed over the fracture. Furthermore, the laboratory experiments demonstrate that the bridges can even hold the sample cut through by a fracture together, in one piece. In order to investigate this phenomenon, we model constricted fracture with bridges as a crack with Winkler layer. The stiffness of the Winkler layer is controlled by the bridge geometry and distribution. The model shows that short constricted fractures are insignificantly different from the conventional cracks; only large fractures, i.e. the fractures whose size is of the order of the characteristic scale of the bridge constriction are affected. The characteristic scale of constriction is inversely proportional to the equivalent bridge stiffness. The constricted fractures have the opening and the stress intensity factors bound as the fracture dimensions proportionally increase, which distinguish them from the conventional cracks where both the opening and the stress intensity factors tend to infinity as the crack size increases. The model proposed can improve our understanding of both natural cracks and large hydraulic fractures.

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Title: Optimal Multi-Level Monte Carlo Methods for the Stochastic Drift-Diffusion-Poisson System and for Stochastic Homogenization

Author(s): Leila Taghizadeh, Amirreza Khodadadian, Stefan Rigger, *Clemens Heitzinger, *TU Wien*.

The numerical solution of stochastic homogenization problems and of stochastic partial differential equations faces the computational problem that usually many samples are required, while each sample is the solution of a (deterministic) partial differential equation. Furthermore, numerical algorithms for these problems generally depend on parameters that must be determined. We have therefore been developing optimal numerical problems for leading model problems that minimize the overall computational cost for a prescribed total error. The first model problem is the numerical stochastic homogenization of elliptic problems, and in particular the numerically demanding case where the permittivity is a piecewise constant function modeling randomly placed and sized inclusions in a background medium [1]. The second model problem is a system of SPDE, namely the stochastic drift-diffusion-Poisson system, which provides a general description of charge transport in random environments [2]. A real-world application are the effects of random dopants in nanoscale transistors or sensors, the limiting factor in current transistor technology. The numerical approach is the following. We derive estimates for the total error by splitting it into its components and we model and measure the computational work as a function of the as yet unknown discretization parameters. In order to determine the discretization parameters, a nonlinear constrained optimization problem is then stated for the minimization of the total computational work for a prescribed total error. The details of optimal numerical algorithms for the two sample problems are discussed and numerical results are presented. In the case of the numerical stochastic homogenization of elliptic problems, recent improvements compared to our previous work [1] are discussed. The goal is a fully automatic and optimal algorithm. In the case of the stochastic drift-diffusion-Poisson system, we present improvements to our recent work [2]. The latest algorithm is an optimal multi-level randomized quasi Monte Carlo method. Simulation results of a realistic nanowire device and a comparison with measurements are presented as well. References [1] Caroline Geiersbach, Clemens Heitzinger, and Gerhard Tulzer. Optimal approximation of the first-order corrector in multiscale stochastic elliptic PDE. SIAM/ASA J. Uncertainty Quantification, 4(1):1246–1262, 2016. [2] Leila Taghizadeh, Amirreza Khodadadian, and Clemens Heitzinger. The optimal multilevel Monte-Carlo approximation of the stochastic drift-diffusion-Poisson system. Computer Methods in Applied Mechanics and Engineering (CMAME), 318:739–761, 2017.

14th U.S. National Congress on Computational Mechanics
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Title: hp-Finite Element Modeling of Silicon Solidification

Author(s): *Brian Helenbrook, *Clarkson University*.

An arbitrary-Lagrangian-Eulerian hp finite element formulation for predicting the solidification of silicon is presented. This method uses an unstructured mesh with local mesh adaptation so that large changes in the interface shape can be simulated. Test cases show that optimal orders of accuracy (p+1, where p is the polynomial degree used on each element) can be obtained using this formulation. Solidification kinetics are included to model the non-isotropic growth of solid silicon. These kinetics include 2D nucleation, faceted growth, and roughened growth effects. Results are shown for the growth of an instability which eventually forms [111] growing facets.

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Title: Modeling Surface Soil Erosion by Water Using SPH

Author(s): *Elizabeth Hernández Zubeldia, *Lutheran University of Brazil*; Georgios Fourtakas, Benedict D. Rogers, *University of Manchester*; Márcio M. Farias, *University of Brasilia*.

Sediment scouring and suspension due to liquid flows are examined in the context of modeling the onset of erosion as the fluid creates a shear layer of sediment over the sediment bed. The problem is analyzed using the Smoothed Particle Hydrodynamics (SPH) which is a Lagrangian simulation method where particles move according to governing dynamics. Its major advantage is the absence of a mesh, making it ideal for problems involving the large nonlinear sediment motions and mixing that occurs during soil erosion. In this work, a new treatment of the suspension of the sediment in water channels is presented employing the Shields theory to extend the state-of-the-art two-phase SPH model for rapidly varying flows [1]. Turbulence at the interface is represented through a log-law in a similar approach to Manenti et al. [2]. For an accurate model of erodible beds, the Shields erosion criterion is combined with the Drucker-Prager yield criterion. These two criteria have been combined to exploit the ability of the model to simulate both the entrainment of soil by water and the dynamics of the subsurface soil material. SPH simulations can be computationally expensive. To accelerate the computation and to allow for realistic modelling of flows where the length-scales are large in comparison to the interface, the multi-phase model formulation has been implemented into DualSPHysics GPU solver [www.dual.sphysics.org]. The capability of the new approach is demonstrated by simulating a 2-D dam break experiment over erodible bed initially using the Shields and Drucker-Prager erosion criteria separately in order to compare the behavior of the isolated criteria. The experiment is then modeled using the combined approach herein presented. Satisfactory qualitative agreement between the numerical model and experimental results is observed representing an improvement over the state-of-the-art. References: [1] Fourtakas, G. and B. D. Rogers. 2016. “Modelling Multi-Phase Liquid-Sediment Scour and Resuspension Induced by Rapid Flows Using Smoothed Particle Hydrodynamics (SPH) Accelerated with a Graphics Processing Unit (GPU).” Advances in Water Resources. Retrieved (http://linkinghub.elsevier.com/retrieve/pii/S0309170816300926). [2] Manenti, S., S. Sibilla, M. Gallati, G. Agate, and R. Guandalini. 2012. “SPH Simulation of Sediment Flushing Induced by a Rapid Water Flow.” Journal of Hydraulic Engineering 138(3):272–84.

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Title: On the DPG Method and Non-Standard Boundary Conditions

Author(s): Thomas Führer, *Norbert Heuer, *Universidad Catolica de Chile*; Michael Karkulik, *Universidad Tecnica Santa Maria*; Ernst p. Stephan, *Leibniz Universität Hannover*.

The discontinuous Petrov-Galerkin method with optimal test functions aims at discretizations that automatically satisfy the discrete inf-sup condition. In contrast to the Galerkin finite element method, there are some specific difficulties to incorporate boundary conditions, in a wider sense, that are non-standard. Here, we think of transmission conditions and the coupling with boundary elements, or contact conditions that give rise to variational inequalities. We discuss the connection of the DPG method with mixed formulations and saddle point problems, and present an abstract framework [1] that allows to deal with the aforementiond transmission [1,2] and contact conditions [3]. We gratefully acknowledge support by Fondecyt-Chile through project 1150056. [1] T. Fuehrer, N. Heuer, M. Karkulik: On the coupling of DPG and BEM. Mathematics of Computation, appeared online. [2] T. Fuehrer, N. Heuer: Robust coupling of DPG and BEM for a singularly perturbed transmission problem. Computers and Mathematics with Applications, appeared online. [3] T. Fuehrer, N. Heuer, E. P. Stephan: On the DPG method for Signorini problems. arXiv:1609.00765, 2016.

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Title: Robust, Efficient, and Geometrically Flexible: Entropy-Stable High-Order Summation-By-Parts Discretizations on Simplex Elements

Author(s): Jared Crean, *Jason Hicken, *Rensselaer Poly. Institute*; David Del Rey Fernández, Mark Carpenter, *NASA Langley Research Center*; David Zingg, *University of Toronto*.

High-order summation-by-parts (SBP) discretizations can be constructed that are entropy stable, and this provides a form of nonlinear stability for simulations of gas dynamics. However, classical SBP methods are based on finite-difference operators that are limited to tensor-product blocks/elements. In this talk, we present our work in extending entropy stability to recently proposed multidimensional SBP operators, which permit greater flexibility in the mesh generation process. In the absence of numerical dissipation, we prove that these generalized SBP discretizations can be made entropy conservative without sacrificing primal-variable conservation or accuracy. The theoretical results are verified using simplex elements applied to the isentropic vortex and the Taylor-Green vortex.

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Title: Characterization and Prediction of Random Short-Fiber Reinforced Composite Properties

Author(s): *Mason Hickman, Prodyot Basu, *Vanderbilt University*.

The current emphasis on performance driven design approaches requires a more critical look toward realizing the relationship between material constituents and structural performance, as the global response of composites is controlled by the characteristics of the constituent phases and their interfaces at the meso- or microstructural level. Multiscale design methods have been introduced in which optimal microstructure processing techniques and characteristics are identified to achieve a target macroscale response for a range of random heterogeneous materials. Fundamental to this approach is the identification of a quantitative relationship between microstructure composition and material performance. This enables intelligent tailoring of a mix of material phases of different types, shapes, and sizes to satisfy the needs of a particular application in terms of performance, cost, and ease of manufacture. A 2-phase random short-fiber reinforced composite with matrix inelasticity and damage is considered. The matrix is a brittle ceramic with a small volume fraction (<2%) of ductile fibers added to provide improved strain energy capacity in tension. Factors influencing the coarse scale behavior of such composites are discussed, including phase volume fraction, diameter, strength, length, distribution, and the interfacial bond characteristics of the constituents. Methods for characterizing the random material microstructure are detailed. A correlation function is introduced for predicting the response of a random short-fiber reinforced composite based on probable damage paths. Microstructural descriptors are mapped to composite material properties by stochastic process.

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Title: Basic Study on Hydroelastic Slamming Simulations by a Fully-Lagrangian Coupled MPS Method

Author(s): *Takefumi Higaki, Masashi Kashiwagi, *Osaka University*; Abbas Khayyer, *Kyoto University*; Jong-Chun Park, *Pusan National University*.

As a ship becomes larger, hydroelastic effects of slamming will be more significant. Hence, precise calculation of such effects is of significant importance and accordingly robust computational methods should be developed. Because of fully Lagrangian meshfree nature, particle methods are inherently well suited for Fluid-Structure Interactions (FSI) involving large deformations. Thus, in this study, a fully Lagrangian coupled computational method [1] is modified and applied to the simulation of hydroelastic slamming. The method applied is based on MPS (Moving Particle Semi-implicit) method with a consistent coupling scheme for fluid and structure solvers. Two benchmark tests are conducted as a basic study on hydroelastic slamming: one is a wedge-drop test compared with a semi-analytical solution, and the other is a panel-drop test corresponding to the experiments by Allen [2]. Among several enhanced schemes, Weak Compressibility, which treats the fluid as weakly compressible with physical speed of sound, plays a great role in stabilizing slamming-induced hydrodynamic pressures. In order to improve the numerical results, a so-called collision model should not be used although it is a commonly-used numerical technique, which stabilizes calculations. This scheme does not have a strong physical background. Thus, instead of collision model, a new method based on Corrected MPS (CMPS) [3] is proposed in this study. CMPS satisfies conservation of momentum by considering repulsive (anti-symmetric) inter-particle forces. However, incorporation of CMPS may alter Taylor-series consistency in the presence of particle irregularities or interfaces (e.g. free-surface). Thus, in this study, a combination of corrected Taylor-series consistent pressure gradient model and CMPS is utilized. The required repulsive CMPS-based forces are calculated dynamically as a function of instantaneous flow field and then added to the main pressure gradient model to avoid particle interpenetration. This scheme is thus referred to as "Dynamic CMPS". Improvements are seen in the pressure calculation by using Dynamic CMPS. References: [1] S.C. Hwang, A. Khayyer, H. Gotoh and J.C. Park, Journal of Fluids and Structures, 50, 497-511, 2014. [2] T. Allen. "Mechanics of flexible composite hull panels subjected to water impacts", Ph.D. Dissertation ResearchSpace@ Auckland, 2013. [3] A. Khayyer and H. Gotoh, Coastal Engineering Journal, 50, 179-207, 2008.

14th U.S. National Congress on Computational Mechanics
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Title: DG Methods, Wave Propagation, and Geostrophic Adjustment in Geophysical Fluid Flows

Author(s): *Robert Higdon, *Oregon State University* .

Large-scale motions of the ocean and atmosphere are typically in a state of geostrophic balance, in which the effect of the earth's rotation causes the direction of fluid flow to be orthogonal to the pressure gradient. If a flow is not in such a balance, then it can adjust to a balanced state via propagation of inertia-gravity waves away from the location of imbalance. Recent investigations suggest that discontinuous Galerkin (DG) methods can give much more accurate simulations of this process, compared to traditional finite difference methods. This is indicated in part by dispersion relations, which for DG methods are highly accurate over the entire range of admissible wavenumbers. Numerical experiments in an idealized setting confirm the predictions from the dispersion relations. This talk will include the construction of a test problem involving a multi-layer fluid, for which geostrophic adjustments can be seen both in the fast external mode and in the slower internal modes.

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Title: Non-Conforming Naturally Stabilized Nodal Integration

Author(s): *Michael Hillman, *The Pennsylvania State Univers*; J. S. Chen, *University of California, San Diego*.

Nodal integration is typically employed in the reproducing kernel particle method (RKPM) to yield a truly meshfree method suitable for modelling extremely large deformations. However, stability of nodal integration is difficult to achieve without introducing additional evaluation points or higher-order derivatives which are both computationally expensive. Further, user-tuneable parameters are sometimes needed, which is of course undesirable. In this work, a non-conforming naturally stabilized nodal integration is introduced to circumvent these issues. Taylor expansion of strains with implicit gradients in naturally stabilized nodal integration (NSNI) [1] yields a stabilized nodal integration with high computational efficiency, with the cost essentially the same as direct nodal integration. Stabilization constants also arise naturally rather than tuneable parameters. The method is cast under a non-conforming strain smoothing framework [2] to achieve additional stability and robustness in semi-Lagrangian RKPM. The method is totally devoid of expensive meshfree derivatives, which further enhances efficiency and ease of implementation of NSNI. Simulation of extreme events such as penetration problems and landslides will be presented to demonstrate the effectiveness of the proposed framework for modelling extremely large deformation problems. REFERENCES: [1] M. Hillman, J. S. Chen, "An accelerated, convergent, and stable nodal integration in Galerkin meshfree methods for linear and nonlinear mechanics," Int. J. Numer. Methods Eng. 107, 603–630, (2016);[2] J. S. Chen, W. Hu, M.A. Puso, Y. Wu, X. Zhang, "Strain smoothing for stabilization and regularization of Galerkin meshfree methods," Lecture Notes in Computational Science and Engineering, Vol. 57, 57–75, Springer, Berlin, (2007).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Non-Differentiable Energy Formulation with Nitsche Flux for Time-Continuous Cohesive Fracture

Author(s): *M. Reza Hirmand, Katerina D. Papoulia, *University of Waterloo*.

The proposed energy minimization formulation of initially rigid cohesive fracture rests on a cohesive potential that is non-differentiable at the origin. A consequence of the non-differentiability is that there is no need to define an activation criterion. This makes the method amenable to implicit time stepping, since the activation criterion no longer interacts with the nonlinear solver. The non-differentiability is treated with a continuation method in which the initially rigid behaviour is achieved via solving a sequence of problems corresponding to an initially elastic model. The continuation method drives the model to initially rigid behavior to desired accuracy. The Nitsche method is used to write the constrained objective potential without the need of introducing Lagrange multipliers as additional unknowns. The minimal energy configuration is obtained by making use of the trust region algorithm which is able to handle the non-convex objective potential resulting from cohesive interfaces. The proposed approach greatly simplifies the implementation of initially rigid cohesive models avoiding the issue of discontinuous forces observed in the previous literature. It is shown through numerical experiments that the method exhibits convergence in velocity norms when the time step is refined. References: Lorentz, E. (2008). A mixed interface finite element for cohesive zone models. Computer Methods in Applied Mechanics and Engineering, 198(2), 302-317. Papoulia, K. D. (2017). Non-differentiable energy minimization for cohesive fracture. International Journal of Fracture, 204(2), 143-158.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Numerical Analysis for Diffusion-Induced Cracks

Author(s): *Sayako Hirobe, Kenji Oguni, *Keio University*.

The moisture/thermal diffusion in the materials results in the inhomogeneous shrinkage of the materials. This inhomogeneous shrinkage produces the excessive stress and the fracture. The diffusion-induced cracks are easily observed in nature such as the drying soil fields and the columnar joint. These cracks form particular patterns depending on the materials and the conditions. The basic features of these crack patterns have been intensively studied with various materials and conditions. The results of these experimental studies show that the pattern of the diffusion-induced cracks has the typical length scale with typical geometry and this typical length scale changes systematically depending on the experimental conditions. These basic features imply the existence of the common governing mechanism for the pattern formation of the diffusion-induced cracks. Though the previous numerical studies have made an effort to model the diffusion-induced cracks and reproduce their particular patterns, the model applicable to the various crack patterns has not been proposed yet. In this research, the problem of the diffusion-induced cracks is modeled as the coupling of moisture/thermal diffusion, deformation of the materials, and fracture in the framework of the continuum mechanics. In this model, the diffusion problem and the deformation problem have the strong discontinuity due to the development of the fracture. To solve this multi-physics problem with the strong discontinuity, we perform the weak coupling analysis of FEM and PDS-FEM (Particle Discretization Scheme Finite Element Method). PDS-FEM is a fracture analysis method which can treat the deformation and the fracture seamlessly without introducing the additional nodes and re-meshing. Through the numerical analysis, we reproduce the pattern formation process of the diffusion-induced cracks and the systematic change of the crack patterns depending on the conditions. The results of this numerical analysis show the satisfactory agreement with the experimental observations. References: [1] S. Hirobe, K. Oguni, Coupling analysis of pattern formation in desiccation cracks, Comput. Methods Appl. Mech. Engrg. 307 (2016) 470–488. [2] K. Oguni, M.L.L. Wijerathne, T. Okinaka, M. Hori, Crack propagation analysis using PDS-FEM and comparison with fracture experiment, Mechanics of Materials. 41 (2009) 1242–1252.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Estimation of the Remaining Useful Life, Using a Microstructure-Based Life Prediction Model and Probabilistic Prognostics

Author(s): Saikumar Yeratapally, *NIA*; Patrick Leser, *Jacob Hochhalter, *NASA*.

More than 50% of mechanical failures in aircraft components are due to fatigue. Fatigue-induced catastrophic failures of components can be avoided by being able to better predict the remaining useful life of com- ponents, which would ultimately help in the timely replacement and re- pair of components. To predict fatigue scatter, it is important to consider both the geometric complexities of the component and the complex het- erogeneities of the material microstructure, which play a prominent role in fatigue crack initiation (FCI) and the microstructurally small fatigue crack growth (MSFCG). With this as a motivation, a microstructure- based fatigue life prediction model is used to link the variability in the microstructure of the material to the scatter in fatigue life. Variability in the microstructure is captured by statistically-equivalent 3D finite element models, which are generated by sampling known distributions of grain morphology, second phases, and attributes of nearest-neighbor grains. A microstructure-based fatigue life is then computed for each sampled mi- crostructure, from which a probability density function for fatigue life spent in the FCI and MSFCG regimes is estimated. This microstructure- based fatigue life scatter data is then used as input prior distributions by a microstructurally-large fatigue crack growth simulator, which captures the geometric complexities. The total fatigue life is then estimated using Monte Carlo sampling. Once the crack is long enough to be measured via in-situ diagnostics, the overall uncertainty in the total remaining life prediction is systematically reduced via Bayesian inference and Markov chain Monte Carlo sampling.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Part-Level Finite Element Simulation of Selective Laser Melting

Author(s): *Neil Hodge, Robert Ferencz, *LLNL*.

Selective Laser Melting (SLM) is a manufacturing process which can realize significant benefits over traditional manufacturing processes, including significantly shortened time between design and manufacture of parts, and the ability to create parts with much more geometric complexity than has previously been possible or tenable. However, the extreme sensitivity of the results to input parameters results in a process that is difficult to predict, and thus control. Indeed, it is not uncommon for the resulting parts to vary significantly from their as-designed geometry, due to the influence of extreme and inhomogeneous thermal gradients. The goal of this research is to determine the physics needed to represent this problem at the part scale, and to develop the numerical methods necessary to simulate the problem in a timely manner. The first part of the presentation will present a review of the continuum modeling strategies and numerical methods. The current work uses a thermal source originally published by Gusarov, et al., to represent the effect of the laser. The material is considered a multi-physics continuum, with a coupled thermal-solid material model. The thermal model includes features to represent the phase changes, as well as different constitutive parameters to define the behavior of the different solid states (powder vs. bulk). The coupling happens via both the usual mechanisms, as well as the dependence of the material properties on the phase. The second part of the presentation presents studies of the correlation between the numerical solutions and various experimental results. Several experimental configurations have been studied in an effort to characterize the effect of the process parameters on the final part, with the samples being on the centimeter scale. The experimental results derived from these samples will be compared to the simulation solutions, and in particular, residual deformations and stresses will be discussed.

14th U.S. National Congress on Computational Mechanics
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Title: Numerical Simulation of Grain-Scale Mechanics in the Dynamic Compaction of Granular Materials

Author(s): *Michael Homel, *Lawrence Livermore Nat. Lab*.

The physics of packing, force chains, stability, and jamming in granular systems have been widely studied, frequently by modeling the systems as a collection of rigid or elastic bodies. However, the dynamic compaction response of granular systems is less well understood. During compaction the bulk response is governed by grain-scale fracture, fragmentation, comminution, and granular flow, introducing significant complexities that prohibit many assumptions that have been used to understand simpler systems. Mesoscale analysis provides an opportunity to study how the individual grain-scale mechanisms affect the bulk response, but numerical simulation of these mechanisms highly nontrivial. We study the dynamic compaction of packed silica glass beads, for which we have obtained detailed synchrotron-source x-ray imaging of grain-scale fracture, fragmentation, and granular flow under both dry and saturated conditions. In these tests we observe that the presence of a pore-space fluid dramatically changes the fracture propagation in the granular material. We model the experiments the material point method (MPM) using the recently developed damage-field gradient partitioning approach, which has a unique capability to produce mesh-independent predictions of fracture with subsequent comminution and granular flow in brittle materials [1]. Using these capabilities we investigate how the grain material constitutive model, initial contact state, and experimental geometry affect the observable response. This investigation showcases the capabilities of the DFG-partitioning method for mesoscale simulation porous brittle materials and experimentally validates this approach for the study of granular compaction. References: [1] Homel, Michael A., and Eric B. Herbold, "Field gradient partitioning for fracture and frictional contact in the material point method", International Journal for Numerical Methods in Engineering 109.7 (2017): 1013-1044.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Higher Order Space-Time Hybridizable Discontinuous Galerkin Methods for Incompressible Flows on Sliding Meshes

Author(s): *Tamas Horvath, Sander Rhebergen , *University of Waterloo*.

In this talk, we present a Hybridizable Discontinuous Galerkin (HDG) method for incompressible flows around moving objects. One way of dealing with such a problem is to use a mesh that has a part that mimics the movement of the object and another part that is fixed with a sliding boundary in between. We use HDG methods in space that can provide a locally conservative solution while keeping the number of degrees of freedom lower than standard DG methods. DG is used also for the temporal discretization allowing an arbitrarily high order approximation in time. Due to hybridization, the facet variables on the sliding boundary will provide the only connection between the fixed and moving region of the domain. The numerical and scalability tests were carried out using the MFEM library.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Multi-Material Topology Optimization for Energy Absorption Capacity Assuming Finite Elastoplastic Deformation

Author(s): *Hiroya Hoshiba, Junji Kato, Takashi Kyoya, *Tohoku University*.

The present study proposes a topology optimization method to improve energy absorption capacity. This method can be applied to optimal design of structure consisting of multi-phased material assuming finite elastoplastic deformation. Regarding topology optimization considering finite elastoplasticity, a previous work by [1] introduces sensitivity analysis based on the so-called transient adjoint method. However, kinematic hardening behavior in addition to finite strain theory has yet to be considered. In this study, the advanced elastoplastic material model is incorporated into the traditional topology optimization framework. In formulating finite strain elastoplastic model including kinematic hardening law, it is known that back stress rate as an internal variable has crucial instability such as stress oscillation. To avoid this problem, elastoplastic constitutive equations are described with reference to plastic intermediate configuration. This leads to a new formulation for sensitivity analysis, and the optimization algorithm can be operated based on analytically derived sensitivity. Some optimization calculations are carried out to verify practical concerns, e.g. accuracy in sensitivity, computational costs and convergence of optimal solution.
Reference: [1] M. Wallin, V. Jönsson, E. Wingren: Topology optimization based on finite strain plasticity, Struct. Multidisc. Optim. 54: 783-793(2016).

14th U.S. National Congress on Computational Mechanics
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Title: Ventricular, Vascular and Valvular Fluid-Structure Interaction

Author(s): *Ming-Chen Hsu, *Iowa State University*.

The aim of this work is to develop a computational framework for ventricular, vascular and valvular fluid–structure interaction (FSI) simulations. The motivating application is the simulation of heart valve function over the complete cardiac cycle. Due to the complex motion of the heart valve leaflets, the fluid domain undergoes large deformations, including changes of topology. We propose an immersogeometric method that directly analyzes an isogeometric surface representation of the structure by immersing it into a non-boundary-fitted discretization of the surrounding fluid domain. We simulate the coupling of the heart valves and the surrounding blood flow under physiological conditions, demonstrating the effectiveness of the proposed techniques in practical computations. An arbitrary Lagrangian–Eulerian/immersogeometric hybrid methodology is also developed under the augmented Lagrangian framework for FSI. A single computation combines a boundary-fitted, deforming-mesh treatment of some fluid–structure interfaces with a non-boundary-fitted treatment of others. This approach enables us to simulate the FSI of bioprosthetic heart valves implanted in a deforming left ventricle through the entire cardiac cycle.

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14th U.S. National Congress on Computational Mechanics
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Title: A Large Deformation Theory Coupling Photo-Chemical Reaction and Electrochemistry for Light-Responsive Polyelectrolyte Gels

Author(s): *Yuhang Hu, *UIUC*.

The long and flexible polymer chains can be crosslinked to form a three-dimensional network. When the network absorbs a species of small molecules (i.e., a solvent), the existence of the crosslinkers may prevent the polymers from being dissolved. The so-formed aggregate is called gel. When the polymeric network contains functional groups that can undergo photo-chemical reaction, the gel becomes light-responsive. Most photo-chemical reactions in gels will induce a change of the electrochemical properties of the gels, which will cause a change in osmotic pressure and drive the solvent to flow into or out of the network. Accompanying with this process, the gel changes volume and shape dramatically. This behavior renders gels' diverse applications as actuators, sensors, drug delivery agent, etc. To achieve precise control and predictive design in the various applications, in this work we develop a large deformation theory coupling photo-chemical reaction and electrochemistry for light –responsive polyelectrolyte gels. A general framework is introduced. A specific material model is described, including the effects of stretching the network, mixing the polymers with the solvent and ions, polarizing the gel and photo radiation reaction. The theory is used to analyze several materials developed in literature. Good comparison between the theoretical and experimental results is achieved.

14th U.S. National Congress on Computational Mechanics
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Title: Spatial-Temporal Nonlocal Homogenization Model for Transient Wave Propagation in Viscoelastic Composites

Author(s): *Ruize Hu, Caglar Oskay, *Vanderbilt University*.

Heterogeneous materials exhibit complex response patterns when subjected to dynamic loading due to the intrinsic wave interactions induced by reflections and refractions at material constituent interfaces. Controlling these interactions offer tremendous opportunities in many engineering applications. For instance, acoustic metamaterials have received significant recent attention due to the unique and tailorable properties including negative effective density and bulk modulus, and wave attenuation within band gaps. We present a spatial-temporal nonlocal homogenization model for transient wave propagation in elastic and viscoelastic composites. The homogenization model is particularly directed to capturing wave dispersion and attenuation induced by material heterogeneity. The proposed model is derived based on asymptotic homogenization with up to eighth order expansions. A momentum balance equation that is nonlocal in both space and time is consistently derived. Contributions from the high order terms in the momentum balance equation account for the heterogeneity induced wave dispersion and stop band formation. The coefficient tensors of the momentum balance equation are computed directly from microstructural material parameters and geometry. A Hybrid Laplace Transform/Isogeometric Analysis (HLT/IGA) is developed to solve the nonlocal momentum balance equation, which provides global C1 continuity as required by the spatial nonlocal term. The high order boundary conditions are also discussed. Response fields in time domain are obtained by applying discrete inverse Laplace transform method. The performance of the proposed model is assessed against direct finite element simulations and compared to classical homogenization models. The proposed model has demonstrated high level of computational efficiency over direct finite element simulation and accuracy over classical homogenization models. The key contributions of our work are: (1) the proposed model captures the wave dispersion in the first and second pass band and attenuation in the first stop band; (2) all the model parameters are computed directly from the microscale initial-boundary problem as an off-line process; (3) HLT/IGA provides an alternative to solve higher order problems (e.g. gradient elasticity).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Comparing Adult Ribcage Geometries between Populations in the United States and China

Author(s): *Jingwen Hu, Matthew Reed, *University of Michigan*; Peiyu Li, Jinhuan Zhang, *Tsinghua University*.

Background: Thoracic injuries are one of the leading causes of fatalities in motor vehicle crashes. Morphological variations in the human ribcage may affect the thorax impact response and injury tolerance, which have been quantified previously through statistical analyses based on CT scans. However, previous morphological studies focused on the ribcage geometry only for the U.S. population, and studies on rib cortical bone thickness are limited. Therefore, the objective of this study was to quantify the ribcage geometry differences (size, shape, and cortical bone thickness) between the U.S. and Chinese populations. Methods: Anonymous clinical thorax CT scans of 101 adults from the U.S. and 60 adults from China were obtained using a protocol approved by an institutional review board at the University of Michigan. The method for developing the statistical ribcage geometry model has been published previously based on the U.S. subjects. The same method was applied for quantifying the ribcage size and shape for the Chinese subjects, which included landmark identification, Generalized Procrustes analysis, principal component analysis, and regression analysis. A new method was developed to quantify the distribution of rib cortical bone thickness based on clinical CT data. This method calculated the derivative of the Hounsfield Unit values along the rib thickness and estimated the boundary of the rib cortical bone based on local thresholds. For each subject, the rib cortical thickness was measured at 64 sampled locations, and linear mixed model was used to test whether the difference between the U.S. or Chinese populations are statistically significant. Results: In general, the age, sex, height, and BMI effects on ribcage size and shape are consistent between the U.S. and Chinese populations. For example, older or obese subjects tend to sustain flatter rib angle than young or lean subjects regardless of their country. In average, with the same stature, U.S. subjects are with shorter ribcage in height than Chinese subjects, and their coronal view shape is more toward “A” shape compared with the “H” shape presented in the Chinese subjects. The age effect on kyphosis of the thoracic spine is more evident in Chinese than the U.S. subjects. Moreover, the U.S. subjects had significantly thicker cortical bone than the Chinese population by controlling age, sex, and height. Conclusions: This study demonstrated that substantial differences existed in ribcage size, shape, and cortical bone thickness between the U.S and Chinese populations, which may significantly affect their impact responses and injury tolerances.

14th U.S. National Congress on Computational Mechanics
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Title: Bayesian Model Calibration with a Embedded Statistical Characterization of Model Error

Author(s): *Xun Huan, Khachik Sargsyan, Habib Najm, *Sandia National Laboratories*.

Applications of Bayesian model calibration often assume the data are consistently generated from the model---that is, the model is correct. In reality, all models are approximations to the truth. It is thus crucial to quantify and propagate uncertainty induced from the errors in the model due to physical, numerical or structural assumptions. Targeting model predictions with quantified model errors, we introduce a strategy for characterizing model error by embedding a stochastic representation in select model parameters. The embedded approach is particularly advantageous for situations where predictive quantities are the focus: it generates physically meaningful predictions of quantities of interest (QoIs) that automatically respect the governing equations and physical constraints endowed in the model, and provides an intuitive platform for "extrapolating" the model error for predicting new QoIs. The algorithm is also non-intrusive, and treats the model as a black box. Armed with data from higher fidelity sources, we infer model parameters and discrepancy terms simultaneously. The calibration is carried out under a Bayesian formalism, employing the adaptive Metropolis Markov chain Monte Carlo algorithm. The intractable likelihood from this model-error treatment is approximated via various techniques such as Gaussian-marginal approximation and approximate Bayesian computation (ABC). During the calibration procedure, polynomial chaos surrogates are used to replace repeated evaluations of the expensive physical model, and to help facilitate the subsequent uncertainty propagation. We demonstrate our method in large eddy simulations (LES) of supersonic reacting multiphase flow in a scramjet engine, where we study static-vs-dynamic Smagorinsky LES subgrid models, and 2D-vs-3D geometries.

14th U.S. National Congress on Computational Mechanics
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Title: Recursive Integral Eigenvalue Solver with Cayley Transformation

Author(s): *Ruihao Huang, *Michigan Technological Univers*; Jiguang Sun, *Michigan Technological University*.

Recently, a non-classical eigenvalue solver, called RIM, was proposed to compute (all) eigenvalues in a region on the complex plane. Without solving any eigenvalue problems, it tests if a region contains eigenvalues using an approximate spectral projection. Regions that contain eigenvalues are subdivided and tested recursively until eigenvalues are isolated with a specified precision. This makes RIM an eigenvalue solver distinct from all existing methods. Furthermore, it requires no a priori spectral information. In this talk, we implement an improved version of RIM for non-Hermitian eigenvalue problems. Using Cayley transforms, the computation cost is reduced significantly also it inherits all the advantages of RIM. Numerical examples are presented and compared with 'eigs' in Matlab.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Conservation Error Analysis of a Family of Embedded Boundary Methods for Multi-Material Problems with Evolving Domains and Discontinuities

Author(s): *Zhengyu Huang, Charbel Farhat, *Stanford University*.

Embedded (or immersed, ghost) Boundary Methods (EBMs) for Computational Fluid Dynamics (CFD) are gaining popularity, particularly for multi-material flow problems, because they simplify a number of computational issues. These range from meshing the computational domain, to designing and implementing Eulerian-based algorithms for the solution of highly nonlinear fluid-fluid, fluid-structure, and fluid-fluid-structure problems featuring evolving domains and discontinuities, large structural deformations, and even topological changes. However, such methods tend to be at best first-order space-accurate at the material interfaces, and at worst inconsistent at these locations. Because they allow a rigid or flexible moving body to penetrate a fluid mesh - thereby distinguishing between "real" (or "active") fluid nodes that lie in the physical fluid domain, and "ghost" (or "inactive") fluid nodes that lie inside the moving body - they are difficult to analyze mathematically. Using as a backdrop the family of EBMs developed in [1-3] under the name FIVER (FInite Volume method with Exact two-material Riemann problems), this talk presents a methodology for analyzing the performance of EBMs with particular attention to energy conservation. The described methodology highlights the effects of a surrogate material interface and an interpolation or extrapolation performed in the vicinity of such an interface on the local and gloal orders of accuracy of the EBM, and its energy conservation properties. All major results are proved mathematically and demonstrated numerically. References: [1] K. Wang, A. Rallu, J.-F. Gerbeau, and C. Farhat, Algorithms for Interface Treatment and Load Computation in Embedded Boundary Methods for Fluid and Fluid-Structure Interaction Problems, International Journal for Numerical Methods in Fluids, Vol. 67, pp. 1175-1206 (2011). [2] C. Farhat, J.-F. Gerbeau, and A. Rallu, FIVER: A Finite Volume Method Based on Exact Two-Phase Riemann Problems and Sparse Grids for Multi-Material Flows with Large Density Jumps, Journal of Computational Physics, Vol. 231, pp. 6360-6379 (2012). [3] A. Main, X. Zeng, P. Avery, and C. Farhat, An Enhanced FIVER Method for Multi-Material Flow Problems with Second-Order Convergence Rate, Journal of Computational Physics, Vol. 329, pp. 141-172 (2017).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Parallel Adaptive Multigrid Approach to Simulating Phase-Field Problems

Author(s): Feng Wei Yang, *University of Sussex*; *Matthew Hubbard, *University of Nottingham*; Peter Jimack, *University of Leeds*.

This presentation will describe the application of a new software tool, developed for the efficient approximation of systems of parabolic-type partial differential equations with multiscale features, to a phase-field model of tumour growth. The computational performance is achieved by combining an optimally efficient nonlinear multigrid solver with adaptivity in both space and time in a parallel implementation [1]. This allows us to implement implicit time-stepping schemes which have the high level of stability necessary for multiscale simulations, and to resolve small-scale features (such as the diffuse interfaces inherent in phase-field models) with relatively modest computational resources. This software has been applied to a range of problems, but the main focus for this presentation will be on two- and three-dimensional simulations of tumour growth using a phase-field model [2]. The challenges of obtaining scalable parallel performance for a software tool that combines local mesh adaptivity with a multigrid solver will also be outlined. [1] F.W.Yang, C.E.Goodyer, M.E.Hubbard, P.K.Jimack, An Optimally Efficient Technique for the Solution of Systems of Nonlinear Parabolic Partial Differential Equations, Adv Eng Softw, 103:65-84, 2017. [2] S.M.Wise, J.S.Lowengrub, V.Cristini, An Adaptive Multigrid Algorithm for Simulating Solid Tumor Growth Using Mixture Models, Math Comput Model, 53:1-20, 2011.

14th U.S. National Congress on Computational Mechanics
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Title: Computational Vademecum Efficient Simulation of Stokes Flow

Author(s): *Antonio HUERTA, *UPC-BarcelonaTECH*.

Design optimization and uncertainty quantification, among other applications of industrial interest, require fast or multiple queries of some parametric model. The Proper Generalized Decomposition (PGD) provides a separable solution, a computational vademecum explicitly dependent on the parameters, efficiently computed with a greedy algorithm combined with an alternated directions scheme and compactly stored. This strategy has been successfully employed in many problems in computational mechanics. The application to problems with saddle point structure raises some difficulties requiring further attention. Here a PGD formulation of the Stokes problem is proposed. Various possibilities of the separated forms of the PGD solutions are discussed and analysed, selecting the more viable option. The efficacy of the proposed methodology is demonstrated in numerical examples for both Stokes and Brinkman models. Recall that PGD is extremely computational efficient on the online phase, because it does not require solving a reduced or surrogate problem. In fact, only interpolations are performed, which imply fast numerical evaluations. Nevertheless, the offline phase may require extensive computer resources. Here, high-fidelity techniques are proposed to improve accuracy and performance in the offline phase.

14th U.S. National Congress on Computational Mechanics
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Title: Isogeometric Analysis: Past, Present, Future

Author(s): *Thomas J.R. Hughes, *UT - Austin*.

October 1, 2015 marked the tenth anniversary of the appearance of the first paper [1] describing Isogemetric Analysis. Since its inception it has become a focus of research within both the fields of FEA and CAD and is rapidly becoming a mainstream analysis methodology and a new paradigm for geometric design [2]. The key concept utilized in the technical approach is the development of a new paradigm for FEA, based on rich geometric descriptions originating in CAD, resulting in a single geometric model that serves as a basis for both design and analysis. In this overview lecture I will describe some areas in which progress has been made in developing improved Computational Mechanics methodologies to efficiently solve problems that have been at the very least difficult, if not impossible, within traditional FEA. I will also describe current areas of intense activity and areas where problems remain open, representing both challenges and opportunities for future research (see, e.g., [3,4]).
Key Words: Computational Mechanics, Computer Aided Design, Finite Element Analysis, Computer Aided Engineering REFERENCES [1] T.J.R. Hughes, J.A. Cottrell and Y. Bazilevs, Isogeometric Analysis: CAD, Finite Elements, NURBS, Exact Geometry and Mesh Refinement, Computer Methods in Applied Mechanics and Engineering, 194, (2005) 4135-4195. [2] J.A. Cottrell, T.J.R. Hughes and Y. Bazilevs, Isogeometric Analysis: Toward Integration of CAD and FEA, Wiley, Chichester, U.K., 2009. [3] Special Issue on Isogeometric Analysis, (eds. T.J.R. Hughes, J.T. Oden and M. Papadrakakis), Computer Methods in Applied Mechanics and Engineering, 284, (1 February 2015), 1-1182. [4] Special Issue on Isogeometric Analysis: Progress and Challenges, (eds. T.J.R. Hughes, J.T. Oden and M. Papadrakakis), Computer Methods in Applied Mechanics and Engineering, 316, (1 April 2017), 1-1270.

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14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Two-Way Integration of Mesh Adaptivity with High-Deformation Multi-Material Simulation

Author(s): *Daniel Ibanez, Thomas Voth, *Sandia National Laboratories*; Glen Hansen, .

We present progress in tightly integrating adaptivity within the time stepping loop of a Lagrangian hydrodynamics simulation with complex evolving geometries. This introduces the need for the more sophisticated size field and solution transfer algorithms we present, which are examples of the simulation's influence on the adaptation code. Metric field satisfiability needs to be maintained by controlling metric gradation as the field is advected, and also by responding to evolving geometric constraints on maximum element size. We also present cases in which adaptivity can inform the Lagrangian simulation, by detecting proximity and acute angles in evolving geometry problems. These situations may trigger the use of dedicated small-scale models to avoid approaching infinitely small elements and time steps. Several example simulations will demonstrate how this sophistication quickly becomes necessary even in simple cases of Lagrangian multi-material deformation.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Reduced Order Strategy for Transient Problems with High Moving Gradients

Author(s): *Sergio Idelsohn, *ICREA-CIMNE, Barcelona, Spain*; Alejandro Cosimo, Alberto Cardona, *CIMEC-CONICET-UNL, Santa Fe, Argentina*.

The aim of this presentation is to solve parabolic problems with highly concentrated moving gradients. A naive approach to tackle this kind of problems would be to refine the mesh as much as needed in all the regions of the domain that are in the vicinity of the path of the moving gradient. One alternative is to adaptively refine the mesh following the moving gradient. Despite the fact that previous options are valid, both are very expensive and they are not so friendly to the formulation of Reduced Order Models (ROMs) because they do not help to tackle the space-time coupling of such problems [1]. The alternative proposed in this presentation is to adopt a global/local scheme, in which a moving local fine mesh describes the neighborhood of the moving gradient and a coarse global mesh describes the analysis domain. In order to glue the two meshes a number of Lagrange multipliers are added to the boundary contour of the fine mesh [2]. It should be noted that the boundary of the fine domain does not need to conform to the elements' boundary of the coarse domain. The big advantage of the proposed strategy is the possibility to reduce drastically both: the fine mesh Degrees of Freedom (DOF) and the Lagrange multipliers DOF, avoiding the space-time coupling problem existing in the global solution. Only transient heat conduction with a concentrated moving heat source are treated in this presentation but the strategy may be generalized to more complex problems with vectorial unknowns like the Navier-Stokes equations. In a series of numerical examples, it is shown that POD modes may be obtained training the problem in one part of the domain and then, to use only a few of these POD modes to solve problems with the gradients in different areas without significant variations of the relative error. References [1] A. Cosimo, A. Cardona, S. Idelsohn, “Improving the k-Compressibility of Hyper Reduced Order Models with Moving Sources: Applications to Welding and Phase Change Problems”, CMAME, 274, 237-263, 2014. [2] A. Cosimo, A. Cardona, S. Idelsohn, “General Treatment of Essential Boundary Conditions in Reduced Order Models for Non-Linear Problems”, AMSES, 3:7, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: A New Accurate Numerical Approach to Wave Propagation, Structural Dynamics and Heat Transfer Problems

Author(s): *Alexander Idesman, *Texas Tech University, USA*.

A new numerical approach for computer simulation of the dynamic response of linear elastic structures as well as heat transfer is suggested. It includes two main components: a) a new local truncation error reduction technique for linear finite elements and for high-order isogeometric elements (the order of the local truncation error in space is reduced by a factor of 2 from 2p to 4p where p – is the order of the polynomial approximation); these new elements can be equally applied to wave propagation and heat transfer problems, and b) a new two-stage time-integration technique which includes a new two-stage solution strategy with the stage of basic computations and the filtering stage, a new exact analytical a-priori error estimator in time for second- and high-order methods; and a new calibration procedure for the quantification and filtering of spurious oscillations; new criteria for the selection of time-integration methods for elastodynamics. In contrast to existing approaches, the new technique does not require guesswork for the selection of numerical dissipation and does not require interaction between users and computer codes for the suppression of spurious high-frequency oscillations. Different discretization methods in space such as the low- and high-order finite elements, the spectral elements, the isogeometric elements, and others can be used with the suggested two-stage time-integration approach. The comparative study of these space-discretization methods for elastodynamics is presented. 1-D, 2-D and 3-D numerical examples show that the new approach yields an accurate non-oscillatory solution for impact and wave propagation problems and considerably reduces the number of degrees of freedom and the computation time in comparison with existing methods. Using the new approach, wave propagation and structural dynamics problems are uniformly solved. The new numerical technique is applied to the analysis of wave propagation in the components of the Split Hopkinson Pressure Bar (SHPB). A good agreement between the numerical and experimental results for wave propagation in the SHPB is obtained at impact loading. We have also applied the new technique to fracture mechanics for the analysis of stresses in members with cracks under impact loading. It is interesting to note that the calculation of the dynamic stress intensity factor for such problems is more accurate with the new approach than with the approaches based on the introduction of the crack tip enrichment functions (e.g., XFEM). Numerical examples also confirm of the significant increase in accuracy of the new technique for heat transfer problems.

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14th U.S. National Congress on Computational Mechanics
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Title: On the Solution of 3D Free Surface Flows Using Enriched Pressure Shape Functions

Author(s): *Florin Ilinca, *National Research Council Cana*; Bruno Blais, *National Research Council Canada*; Kintak Raymond Yu, .

Free surface flows are a topic of interest for many applications such as injection molding, metal casting, liquid dynamics inside reservoirs or marine flow dynamics. Such flows present particular challenges in the presence of gravity as there is an intrinsic incompatibility between the discrete representation of the pressure and the physical behavior at the interface. This paper discusses different implementations of a three-dimensional finite element solution algorithm for solving free surface flows in the presence of gravity. The method uses fixed meshes and therefore the fluid/air interface is generally located inside mesh elements. Simplified techniques for considering the gravity term on interface elements are compared with a more elaborate approach in which the pressure interpolation is enriched such as to represent the discontinuity of the pressure gradient at the interface. For the enriched method the additional pressure degrees of freedom are eliminated at the elementary system level by static condensation. Therefore, the finite element degrees of freedom and the size of the resulting matrix system remain the same, making implementation much easier compared to extended finite element methods. The enriched pressure discretization is first validated on a series of simple free surface flows for which experimental and/or numerical results are available. The first test problem is the collapse of a column of liquid for which experimental measurements are available. The free surface is well captured and mesh refinement studies indicate that the solution depends very little on the mesh element size. The agreement with the experimental measures is very good. The method is then applied to the flow inside a partially filled 2D enclosure subject to a dynamic movement and the results are compared with other published data. The enriched pressure shape functions result in a stable, oscillation free solution and the method is a very efficient way to accurately solve free surface problems without remeshing or mesh refinement. Finally, the solution methods will be compared for the case of partially filled 3D tank subject to a complex dynamic movement.

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Title: Dynamic Mechanical Characterization of Random 3D Structural Polymeric Foams

Author(s): *Axinte Ionita, Brittany Branch, Brian M. Patterson, Brad E. Clements, Alexander H. Mueller, *Los Alamos National Laboratory*; Dana M. Datellbaum, .

Polymeric foams materials can have various applications in engineering. We consider in this work the mechanical aspects of the behavior of a random 3D structural polymeric foam under high dynamic mechanical loading conditions (shock). In the analysis, the microstructure of the foam is extracted from 3D computed micro-tomography. The mechanical response of the polymeric foam is described in terms of deviatoric and pressure response. Using Direct Numerical Simulations (DNS), Finite Element Method (FEM) and concepts of Micromechanics the average foam response to shock is determined. The results are compared with the shock equations for the homogenized case to determine the effect of fluctuating fields of physical quantities due to the randomness of the foam microstructure. LA-UR-17-21505

14th U.S. National Congress on Computational Mechanics
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Title: Benchmark Solutions for Models of Solids Transport in Hele-Shaw Cell

Author(s): *Vadim Isaev, Ivan Velikanov, Dmitry Kuznetsov, *Schlumberger*; Denis Bannikov, Alexey Tikhonov, .

Modeling of solids transport in a Hele-Shaw cell is usually based on the numerical solution of nonlinear transport equation d(w c) / dt + d (w U c) / dx + d (w V c) / dy = 0, where w, c, and U and V are cell width, solids concentration, and solids velocity components, respectively. In different models, velocities U and V may depend on w, c, and other parameters such as gravity acceleration, solids and fluids density, distribution of other slurry species, etc. This nonlinearity enables the modeling of solids accumulation in some regions of the flow domain. We propose a set of benchmark exact solutions designed for the verification of solids transport algorithms: - traveling wave - formation of shock waves with concentration jumps near domain boundaries impermeable for solids - effects of nonlinear settling velocity on the fronts of domains with settling solids - trapped solid particles The limitations of existing transport algorithms are discussed using these solutions. It is shown the discretization approach may introduce artificial rarefaction waves and other artefacts. References: E. Dontsov, A. Peirce. Slurry Flow, Gravitational Settling and a Proppant Transport Model for Hydraulic Fractures. J. of Fluid Mechanics, December 2014.

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Title: On Modeling of Particles Settling in Hele-Shaw Flows of Non-Newtonian Fluids

Author(s): Vadim Isaev, *Maxim Ivanov, Denis Bannikov, Rostislav Romanovskii, *Schlumberger*.

We consider a flow of a non-Newtonian fluid laden with spherical solid particles through a narrow Hele-Shaw cell. In the majority of existing models, the velocity of particles settling is calculated using basic formulas for drag acting on a sphere, with correction factors representing the effect of solids concentration, solids interaction, and wall effects (hindered settling). For non-Newtonian fluids, the drag force depends on apparent fluid viscosity affected by shear rate. The latter comprises two components representing the effect of settling particles and fluid flow under pressure gradient in a Hele-Shaw cell. This study is aimed to derive a consistent approach for settling modeling taking into account both shear rate components and the effect of particles distribution across the cell. It is shown that particles located at different positions across the cell have different settling velocities. Their spatial distribution across the cell has a significant impact on the bank growth rate. An approach for definition and calculation of mean settling velocity is proposed. Validation of the simulation results against experimental data for power-law fluids is performed. References: E. J. Novotny. Proppant Transport, SPE 6813.

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Title: Three-Dimensional High-Order Simulations of Low-Pressure Turbine Blade Cascades

Author(s): *Arvind Iyer, Yoshiaki Abe, Peter Vincent, *Imperial College London*; Freddie Witherden, Antony Jameson, *Stanford University*; Brian Vermeire, *Concordia University*; Ralf-Dietmar Baier, *MTU Aero Engines AG*.

The turbine stages of a jet engine extract energy from exhaust gasses to drive the compressor, fan, and other auxiliary systems. The efficient design of turbine blades is crucial for reducing emissions of CO2 and other greenhouse gasses. Approximately half the weight of a turbine stage comes from the turbine blades. In order to reduce this contribution, modern turbines are designed to use as few blades as possible. A reduction in the number of blades, however, causes greater loading and separation in the aft portion of the blades; introducing complex, unsteady, three-dimensional phenomena, and reduced efficiency. Accurate simulation of unsteady turbulent flow in the vicinity of complex geometric configurations is critical for the improved design of turbine stages, and hence `greener' aircraft that are more fuel-efficient. In this work, we use PyFR, a high-order accurate Python based computational fluid dynamics solver for petascale simulations of flow over low-pressure turbine linear cascades. The rationale behind algorithmic choices, which offer increased levels of accuracy and enable sustained computation at up to 58\% of peak DP-FLOP/s on unstructured grids [1] will be discussed in the context of modern hardware. A range of software innovations will also be detailed, including the use of runtime code generation, which enables PyFR to efficiently target multiple platforms via a single implementation, and in-situ visualization, which enables visual insight extraction at an unprecedented scale by avoiding storage and I/O bottlenecks. [1] Peter Vincent, Freddie Witherden, Brian Vermeire, Jin Seok Park, and Arvind Iyer. 2016. Towards green aviation with python at petascale. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC '16). IEEE Press, Piscataway, NJ, USA

14th U.S. National Congress on Computational Mechanics
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Title: Model Order Reduction and Control Strategies for Flow-Induced Vibration

Author(s): *Rajeev Kumar Jaiman, *NUS, SIngapore*.

Efficient model reduction and control of flow-induced vibration is of a practical importance in a broad range of engineering applications. Successful prediction and control of vibrations can lead to safer and cost-effective structures in aeronautics, offshore and civil engineering. In particular, the need for such prediction and control becomes crucial for high-performance light structures with increased flexibility. For example, asymmetric vortex shedding shed from a bluff body causes a large unsteady transverse load, which in turn may lead to structural vibrations when the structure is free to vibrate. These large vortex-induced vibrations can lead to damage and potential risk to the structures, in particular for ocean structures such as marine risers, subsea pipelines, and cables operating in a complex dynamic environment. The coupled fluid-structure analysis based on high-fidelity computational fluid dynamics (CFD) can reveal a vast amount of physical insight in terms of vorticity distribution, force dynamics, frequency characteristics and phase relations, and the shape of motion trajectory. Despite improved algorithms and powerful supercomputers, the state-of-art CFD-based fluid-structure simulation is less attractive with regard to parametric optimization and the development of control strategies. Model reduction techniques naturally provide the development of adaptive control strategies for fluid-structure interaction and they are aligned with the industry needs on structural life prediction and monitoring via digital computing (e.g., digital twining). The primary focus of this talk is: (i) to discuss an efficient low-order model for flow-induced vibration, and (ii) to demonstrate a feedback active control algorithm based on the dimensionality reduction for unsteady wake flow and fluid-structure interaction. References 1. R.K. Jaiman, N.R. Pillalamarri, and M.Z Guan. A stable second-order partitioned iterative scheme for freely vibrating low-mass bluff bodies in a uniform flow. Computer Methods in Applied Mechanics and Engineering, 301:187–215, 2016. 2. Yao, W. & Jaiman, R. K. (2016) “A harmonic balance technique for the reduced-order computation of vortex-induced vibration,” Journal of Fluids and Structures 65, 313–332. 3. Yao, W. and Jaiman R.K. “Model Reduction and Mechanism for the Vortex-Induced Vibrations of Bluff Bodies”, J. of Fluid Mechanics (2016), Under revision 4. Yao, W. and Jaiman R.K. “Feedback Control of Unstable Flow and Vortex-Induced Vibration Using Eigensystem Realization Algorithm”, J. of Fluid Mechanics (2017), Under review 5. Jaiman, R. K., Guan, M. Z. & Miyanawala, T. P. (2016) “Partitioned Iterative and Dynamic Subgrid-Scale Methods for Freely Vibrating Square-Section Structures at High Reynolds Number,” Computers & Fluids 133, 1–22.

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Title: Multimaterial Topology Design for Optimal Stiffness and Thermal Conductivity Response

Author(s): Ziliang Kang, *University of Illinois*; *Kai James, *University of Illinois at Urbana-Champaign*.

With the development of advanced additive manufacturing, research on topology optimization for multifunctional structures and materials has grown in popularity. These designs often consist of several constituent materials, and exhibit optimal elastic, thermal or electromechanical response, or some combination of the three. We present a novel method for multimaterial topology design for optimal elastic and thermal response. We consider a typical two-dimensional problem in which we optimize the distribution of three distinct candidate materials plus a void phase. The linear elastic displacement and steady-state temperature distribution due to thermal conductivity are solved using separate uncoupled finite element analyses. The material distribution is represented parametrically via a set of coefficient functions which determine the material properties within each finite element. These material properties are obtained from a superposition of the properties (Young's modulus and thermal conductivity) of the candidate materials. The coefficient functions are defined using a form analogous to that of finite element shape functions, with SIMP-like penalization to ensure convergence to a discrete design with no hybrid elements. We optimize the structures for maximum stiffness, while constraining the maximum local temperature along the bottom surface of the structure due to a constant heat flux at the top surface. In this way, the multifunctional structure is designed for a combination of structural stiffness and thermal insulation. We compare these multifunctional designs with structures optimized purely for elastic or thermal performance, to evaluate the impact and analyze the interaction between these two competing design considerations.

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Title: Epsilon-Martensite Start Temperature Modeling Using First-Principles Calculation

Author(s): *Jae Hoon Jang, Heon-Young Ha, Tae-Ho Lee, *KIMS*; Dong-Woo Suh, *POSTECH*.

With regard to the transformation mechanism of austenitic high manganese as well as stainless steel, the prediction of the ε-martensite start temperature is an important consideration in alloys. The ε-martensite start temperature is the temperature at which transformation occurs from the austenite of the face-centered cubic (FCC) structure to the ε-martensite of the hexagonal closed packed (HCP) structure during cooling. In the case of α'-martensite, several models for predicting the transformation starting temperature are available based on various experimental measurements and thermodynamic database. However, in the case of ε-martensite, it is difficult to apply similar models due to the limitation of thermodynamic database. In this study, we compared the experimentally measured ε-martensite start temperatures and the stability of the FCC and the HCP structures according to the first-principles calculation for various compositions reported in the existing literature. Alloys were simulated by applying a coherent potential approximation (CPA) method to simulate a chemical and magnetic disordered structure in the calculations. ε-martensite with paramagnetic state according to the disordered local moment (DLM) model and austenite with antiferromagnetic state at 0K were compared. As a result, it was confirmed that there is a close relationship between the crystal structure stability and the ε-martensite start temperature. Comparing the effects of other substitutional elements, it was found that the elemental effect on the ε-martensite start temperature was mainly determined by the effect of crystal structure stability depending on the free electron density.

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Title: Analyst-Guided Adaptive Simulation at Extreme Scale-- Beyond In Situ

Author(s): *Kenneth Jansen, *University of Colorado Boulder*; Cameron Smith, Mark Shephard, *Rensselaer Polytechnic Institute*; Benjamin Matthews, *NCAR*.

PDE solvers have made enormous progress in scalability, in some cases scaling to millions of processes. In these cases, the time spent pre and post-processing the results may dwarf the actual time spent solving the problem, even for highly non-linear problems like the Navier-Stokes equations. Worse yet, challenging problems may contain such a high degree of geometric and solution complexity that several cycles of mesh generation or mesh adaptation are required before an acceptable solution is reached. If each stage of each cycle is a separate run then this single solution may take weeks due to queueing delay. A script could combine some stages within a single run using files to transfer state between stages, but this will be error prone, and, as with the multi-run approach, suffer from queueing delays. In principle the script can also combine cycles, but, without feedback from visualization and associated problem definition modifications, this process can easily fail. In this talk, we present extreme-scale simulations linking the flow solver (PHASTA), the visualization filter pipeline (ParaView), and mesh adaptation and load balancing (PUMI) components within a single executable. With this capability we execute multi-cycle adaptive analysis driven by feedback from in-situ visualization within a single job. These components may communicate via files or via in-memory data streams. As the scale increases, significant gains are observed for the latter due to the extreme demands that large process counts place upon the filesystem. Performance will be discussed in the context of the computational hardware (KNL and BGQ) and the filesystem (Lustre and GPFS) within the Argonne National Lab computing facility using process/partition counts ranging from O(10^4-10^6).

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Title: Adaptivity for Active Flow Control on a Vertical Tail Rudder Assembly

Author(s): Michel Rasquin, *Cenaero, Gosselies, Belgium*; Cameron Smith, *Scientific Computation Research Center (SCOREC), RPI, Troy, NY*; Riccardo Balin, *Kenneth Jansen, *U. Colorado Boulder, Aerospace Engineering Sciences, Boulder, CO, USA*; Benjamin Matthews, *National Center for Atmospheric Research (NCAR), Boulder, CO USA*.

Virtual shaping for flight control of aerial vehicles is investigated in this work, where aerodynamics performance of conventional control surfaces such as rudder and flaps can be improved over a wide range of operating conditions. A series of numerical flow simulations of a realistic vertical tail of a commercial aircraft, with a tapered swept stabilizer and a rudder, is considered. For such configurations, active flow control is known to have the capacity to augment the streamwise momentum near the rudder suction peak where separation is typically observed to limit rudder effectiveness for high deflection angles. Specifically, in this talk we focus on the mesh adaptation strategies used to establish a grid independent study of the interaction of a cross flow and a single jet. The modeling process begins with a CAD model that precisely matches the model that was tested in the RPI wind tunnel. This includes full resolution of the synthetic jets back to the diaphragm whose vibratory motion alternately expels and inducts fluid. Next, an initial mesh was created with very fine, layered and graded anisotropic elements near the wall. This mesh used refinement boxes to get a moderate resolution of the separation and wake regions. The first simulation used a steady Reynolds-averaged Navier-Stokes (RANS) model to further define the separated flow regions and the wake. The first adaptation refined in a region identified with an error indicator that was based on a combination of solution error estimates and the RANS eddy viscosity. From this adapted mesh, a Delayed Detached Eddy Simulations (DDES) was initiated. While the agreement with the experiment was good, a second adaptation was carried out based on solution error indicators collected from the statistics of the DDES. In this talk we will discuss the adaptive technology, the application just summarized, and the excellent agreement with experiments achieved. Such agreement would not have been possible without the application of adaptivity at extreme scale. For these simulations, a massively parallel, fully implicit, stabilized finite element flow solver (PHASTA) is used to solve the transient, incompressible Navier-Stokes equations. Two unique assets characterize this flow solver: (i) ability to perform anisotropic adaptivity of the initial 3D unstructured finite element mesh, and (ii) strong scaling performance (shown to scale up to 768k cores (3M processes) of a Blue Gene/Q supercomputer). Newer simulations on a third adaptation carried out on KNL will also be discussed.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Kink Band Instabilities in Layered Media

Author(s): Jens L. Wind, Simon P.H. Skovsgaard, *Henrik M. Jensen, *Aarhus University*.

Layered materials compressed parallel to the layers are prone to fail by the development of a kink band instability where the material inside the band rotates relatively to the material outside the band. The failure mechanism is observed in geological materials, fiber composites, wood and laminated media. The absolute value of the critical stress in compression for such materials can be considerably lower (as much a factor 1/5) than the critical load in tension. The critical compressive stress for kink band formation is known to be sensitive to imperfections such as misalignments of the layer orientation relative to the load direction, and to non-linear material behavior of the constituent materials due to plastic deformation. This makes theoretical investigations of kink band formation challenging as they must allow for non-linear behavior of the constituents as deformations evolve into the finite strain regime. Several open issues exist including the post-failure response where broadening of the kink band may occur. Also open issues involving, three-dimensional effects and effects of residual stresses exist. The present work presents experimental observations of kink band initiation in fiber composites using a micro tensile test device in a scanning electron microscope. We also present theoretical investigations of the post-failure response by extension of previous work based on a constitutive model for a layered material implemented in the finite element package Abaqus. Issues that are addressed include the conditions during the formation, localization and rotation of the material inside the kink band in the first stages after its initiation. Also the conditions in a later stage of the post-failure regime are addressed where the rotation of the material in the band stops, and instead overall deformation of the layered material takes place by a steady-state broadening of the already developed band. References: [1] H.M. Jensen and J. Christoffersen, Kink Band Formation in Fiber Reinforced Materials. Journal of the Mechanics and Physics of Solids 45, 1121-1136, 1997. [2] H.M. Jensen, Analysis of Compressive Failure of Layered Materials by Kink Band Broadening. International Journal of Solids and Structures 36, 3427-3441, 1999. [3] J.L. Wind, A.M. Waas and H.M. Jensen, Initiation of Failure at Notches in Unidirectional Fiber Composites. Composite Structures 122, 51-56, 2015.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Numerical Analysis of Fracture Evolution Using Nonlocal Models

Author(s): *Prashant Jha, Robert Lipton, *LSU*.

We calculate the convergence rate of finite difference and finite element approximations for a class of nonlocal fracture models motivated by peridynamics [5]. We consider force interactions characterized by a double well potential. We show the existence of a regularized model with evolving displacement field in either Holder space or Sobolev space. The rate of convergence of the approximations depend on the ratio of discretization length to the length scale of nonlocal interaction. It is shown that this convergence rate holds for both the forward Euler scheme as well as general single step implicit schemes. The Holder and Sobolev evolutions converge to a brittle fracture evolution in the limit of vanishing nonlocality [1,2,3,4]. References: [1] P. Jha and R. Lipton, Numerical Analysis of Nonlocal Fracture Models in Holder Space, arXiv:1701.02818v3 [math.NA] 25 Jan 2017. [2] P. Jha and R. Lipton, Finite Element Analysis of Nonlocal Fracture Models, Preprint, April 2017. [3] R. Lipton, Dynamic brittle fracture as a small horizon limit of peridynamics, Journal of Elasticity, 117, pp. 21–50 (2014). [4] R. Lipton, Cohesive dynamics and brittle fracture, Journal of Elasticity, 124, Issue 2 (2016), pp. 143-191. [5] S. A. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, Journal of the Mechanics and Physics of Solids, 48 (2000), pp. 175–209.

14th U.S. National Congress on Computational Mechanics
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Title: Numerical Analysis of Nonlocal Fracture Models

Author(s): *Prashant Jha, Robert Lipton, *Louisiana State University*.

In this talk, we present the numerical analysis of a bond-based peridynamic model. Model is nonlinear and is characterized by two wells. One well, near zero strain, correspond to the linear elastic interaction whereas second well corresponds to the softening of material. We present finite element analysis when the solution is in C^1 and C^2. We also analyze the finite difference approximation when the solution is in H\"{o}lder space. We consider H\"{o}lder space as it allows fields which do not have well-defined derivatives. We show that $O(h^2/\epsilon^2)$ is the rate of convergence when the solution is in C^2 and $O(h^\gamma/\epsilon^2)$ when the solution is in H\"{o}lder space. h is the size of mesh, ϵ is the size of the horizon, and $\gamma\in (0,1]$ is the H\"{o}lder exponent. We show that the instability in the peridynamic model is due to softening of bonds and occurs when sufficiently large number of bonds have strain above critical strain. We also consider the model in one dimension. We show that the solution of peridynamic model converges to the solution of elastodynamic. The same is shown for the approximation of peridynamic model. We present some numerical results to verify the claims. This is a joint work with Dr. Robert Lipton.

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Title: Three-Dimensional Computational Framework with Embedded Weak Discontinuities for Shear Localization under Dynamic Loading Conditions

Author(s): *Tao Jin, Hashem Mourad, Curt Bronkhorst, *Los Alamos National Laboratory*.

Shear localization is often observed in metals as a precursor to failure, and characterized by the concentration of plastic deformation within thin bands of material [1]. In this talk, we present an explicit finite element formulation for the treatment of shear localization of rate-sensitive metallic materials under severe dynamic loading conditions. The embedded weak discontinuity approach is adopted to simulate the material behavior under 3-D finite deformation, thus avoiding the need of resolving shear band explicitly. The mechanical threshold stress (MTS) model is modified to include the material softening mechanism introduced by dynamic recrystallization (DRX). The modified MTS model is adopted to characterize the evolution of the material flow stress. Due to the competing effects of hardening and softening mechanisms in rate-sensitive materials, the criterion for the initiation of shear localization is adapted from the J2 flow theory, instead of performing the classical stability analysis based on acoustic tensor. The corotational formulation of the elasto-viscoplasticity and the stress update algorithm are provided to obtain a rotation-neutralized description of the constitutive equations [2]. By comparing the numerical results with the experimental data obtained from different dynamic experiments, we demonstrate the capabilities of the presented computational framework to treat shear localization under severe dynamic conditions. References: [1] Bronkhorst CA, Cerreta EK, Xue Q, Maudlin PJ, Mason TA, Gray III GT (2006) An experimental and numerical study of the localization behavior of tantalum and stainless steel. Int J Plast 22:1304–1335. [2] Mourad HM, Bronkhorst CA, Livescu V, Plohr JN, Cerreta EK (2017) Modeling and simulation framework for dynamic strain localization in elasto-viscoplastic metallic materials subject to large deformations. Int J Plast 88:1–26.

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Title: Experimental and Computational Analysis of the Ballistic Properties of SiC Tile Encapsulated Composite Armor System

Author(s): *ILGUK JO, Seungchan Cho, Sang-Kwan Lee, Sang-Bok Lee, *Korea Institute of Materials*; Minhyung Lee, *Sejong University*.

The response of multilayered composite/silicon carbide tile/composite and SiC tile encapsulated composite targets to high impact velocity more than 1.3km/sec and penetration has been investigated through finite element simulations. SiC and boron carbide particulates were used as a reinforcement material and different aluminum alloys were used as matrix in the composite plate. A high volume fraction of SiC or B¬4C reinforced Al composite plates were produced by a liquid pressing process. The mechanical properties of composites were evaluated for selecting the front and the back plate of the ceramic tile. Both experimental and numerical methods were performed for understanding ballistic properties of developed armor system. For numerical study, LS-Dyna was used as solver with Lagrangian Scheme based on Johnson-Holmquist 2 (JH-2) model. According to the depth of penetration (DOP) by simulation and high velocity impact test, the performance evaluation of the MMC applied armor system has been made by comparing with the conventional systems. The reasonable correlation of models with experimental impact test shows the validity of the present approach for studying ballistic properties of composite armor system. The results indicate that SiC ceramic tile encapsulated by composite has smaller depths of penetrations as compared with SiC ceramic tile and multilayered composite-tile system. Due to the confinement effect in the target, the dynamic damage in the tile encapsulated composite system was lower than other target material.

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Title: Immersed Boundary Method with Spring Network Model for Predicting Vesicle Dynamics in Fluid Flow

Author(s): *Junhong Jo, Do Wan Kim, *Inha University*; Tae-Rin Lee, *Advanced Institutes of Convergence Technology, Seoul National University*.

Immersed boundary (IB) method has been used to simulate various fluid-structure interactions. The main issue is how we efficiently define the mechanics of immersed body. Related to this, spring network model is a simple way to include deformable bodies in the IB method by connecting material points with spring networks. In this presentation, we recruit a spring network model in the IB method for predicting various interactions of deformable cells in shear flow. First of all, fluid-rigid body interaction force in the proposed method is tested by simulating single sphere falling in a channel. The terminal velocity data of sphere in related experiments are compared with the current simulation results. Secondly, we predict the deformation of single cell with linear and nonlinear material properties in a simple shear flow. Finally, we expand the model for multiple interactions among cells in fluid flow. Then we will demonstrate blood flow simulation in complex geometry by using the proposed method.

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Title: Robust and Efficient Validation of the Linear Hexahedral Element

Author(s): *Amaury Johnen, Jean-françois Remacle, *UCL (Belgium)*; Jean-christophe Weill, *CEA (France)*; Thomas Toulorge, *MINES ParisTech (France)*; Christophe Geuzaine, *ULg (Belgium)*.

Among the different types of meshes hexahedral meshes are often desired for the many better properties they offer, such as alignment with physical features or a lower computational cost. They are however by far much harder to generate than tetrahedral meshes. One reason is the fact that robustly asserting the validity of a linear hexahedral element is still an open problem (Ushakova, 2011). Currently, many mesh generators only compute the Jacobian determinant at the 8 nodes of the hexahedra, which is known to be insufficient since the mapping is trilinear (Knupp, 1990). Regarding the quality, the scaled Jacobian is commonly considered by the hexahedral community. The scaled Jacobian is also often only computed on the corners of the hexahedra and it is unclear if it is sufficient to judge their quality. We present a method to robustly assert the validity of the hexahedra by computing the minimum of the Jacobian determinant. The algorithm is based on a previous work presented by Johnen et al. (2013) and is efficient. The same algorithm is adapted to compute the minimum of two quality measure: the scaled Jacobian and another quality measure that is equivalent to the inverse of the condition number.

14th U.S. National Congress on Computational Mechanics
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Title: Three-Dimensional Overhang-Constrained Topology Optimization for Additive Manufacturing

Author(s): *Terrence Johnson, Andrew Gaynor, *U.S. Army Research Laboratory*.

Additive manufacturing (AM) introduces design freedoms that are not available in manufacturing structures from traditional methods. Topology optimization (TO) can design to complex freedoms afforded by AM to produce structures that better satisfy prescribed objectives and constraints. However, there remains limitations on manufacturable topologies due to, for example, the need for sacrificial support material in printed parts. Sacrificial support material, while beneficial in production, can lead to structural damage, surface crack initiators and trapped material. This work proposes a 3D TO design methodology for developing sacrificial support-free structures. Drawing upon observations seen in manufacturing overhang-constrained 2D topologies1, the 3D algorithm is further developed in order to specify nonequal angles in different directions (e.g. 45 degree overhang in all directions except that of the recoating direction). This is accomplished through unique mapping routines in which the shape of the search region is manipulated to suit each particular AM methodology. This approach begins to tackle the problem of simultaneous part design and orientation, which is an area ripe for exploration. Finally, the algorithm is “inverted” in order to design for internal void-free topologies. In this approach, the void regions must “grow” from a certain direction. This last capability has potential to design for additively manufactured molds for casting applications. Reference: 1. Gaynor, Andrew T., and James K. Guest. "Topology optimization considering overhang constraints: Eliminating sacrificial support material in additive manufacturing through design." Structural and Multidisciplinary Optimization 54.5 (2016): 1157-1172.

14th U.S. National Congress on Computational Mechanics
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Title: A Variationally Bounded Scheme for Allen-Cahn Phase Field Equation for Modeling of Two-Phase Flows

Author(s): *Vaibhav Joshi, Rajeev Jaiman, *NUS, Singapore*.

A novel variational method has been proposed to solve the convection-diffusion-reaction (CDR) equation which forms the most canonical form of any physical process ranging from Navier-Stokes flow, Allen-Cahn phase-field to turbulence transport. Solving these equations numerically through discretization introduces spurious oscillations due to inability of the mesh to resolve the crucial subgrid scales. The present positivity preserving variational (PPV) method [1] is aimed to provide a bounded and positivity preserving solution for a broad range of parameters of subgrid-scale physics. A combined GLS-SGS methodology is chosen for the linear stabilization to have minimal phase error via Fourier analysis while consistent nonlinear stabilization is carried out with the help of discrete upwind operation to circumvent Godunov's theorem. At least second order of spatial accuracy is obtained for the method with successful capturing of the internal and boundary layers observed in two dimensions. In the present study, we extend the technique to a conservative Allen-Cahn phase field equation. The order parameter in the phase field equation determines the different phases of the fluid field, whereby unphyiscal oscillations may occur in the order parameter when the convection and reaction effects are dominant. The present method helps to restore positivity in the variable while maintaining boundedness of the phase field equation. By coupling with the Navier-Stokes equation, this PPV-based phase-field solver is then applied for the modeling of two-phase flow. To assess the stability and convergence properties, a systematic parametric study is carried out for increasing complexity of test problems of phase field model. Through numerical experiments, the method is shown to be mass conservative and energy-stable. Finally, canonical cases of two-phase flows are considered for the validation study. This coupling of phase-field with the Navier-Stokes and/or structural equations forms a basis for the integrated analysis of multiphase and fluid-structure interaction within fully-Eulerian setting. References: [1]. Joshi, V. and Jaiman, R. K., A positivity preserving variational method for multi-dimensional convection-diffusion-reaction equation. Journal of Computational Physics, Under review, (2017). (https://www.dropbox.com/sh/hzevq09hsdahdmr/AABGnVbvdfWswxyqd58K7QFXa?dl=0)

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Title: A Thermodynamically Consistent Level Set Approach for Shock-Induced Alpha-Gamma Phase Transition of RDX

Author(s): *Kartik Josyula, Rahul, Suvranu De, *Rensselaer Polytechnic Institute*.

The mechanisms of strain energy dissipation in shocked crystalline solids include plastic slip and/or polymorphic transformation. While the anisotropic elastic-plastic response of single crystals at high strain rate has been studied, modeling the effects of phase transformation has received less attention. We employ the level set method [1] to study shock-induced α-γ phase transformation in RDX single crystals. Our approach is based on a regularization energy functional [2] that does not require explicit reinitialization. A diffusive regularization flux is introduced to maintain the signed distance property of the level set function. The diffusive flux enables incorporating the level set formulation within Galerkin finite element framework. The level set approach is evaluated using one-dimensional and three-dimensional models of a bar shocked on the (100) plane of RDX. The diffusive form of the flux ensures curvature based motion and hence the level sets around the interface evolve smoothly for both examples. We compared the interface evolution using the proposed scheme with the velocity extension method for the one-dimensional example. The time lag in the interface motion captured by the two schemes decreases along the direction of shock propagation as well as with the element size and the number of Gauss points used. The particle velocity time trace and the stress history compare well between the two schemes. The marginal lag in the particle velocity and stress can be reduced by appropriate choice of the regularization energy. The efficacy of the proposed level set method depends on the choice of the regularization energy and the applied Dirichlet boundary conditions. The parameter in the regularization energy should be carefully chosen to obtain desired results. For the three-dimensional example, the proposed approach is shown to capture the characteristic features associated with the α-γ phase transformation in RDX such as stress relaxation behind the phase interface. We did not observe any slip activity for loading on the (100) plane or due to the α-γ phase transformation. This is consistent with the experimental observations where RDX shocked on the (100) plane undergoes elastic deformation. There were no spatial disturbances observed in the evolution or distribution of the level set parameter, compressive stress, or temperature. The proposed level set approach has simulated a smooth evolution of the α-γ phase interface in shocked RDX. References: [1] Osher and Sethian, J. Comput. Phys. 79, 12 (1988). [2] Li et al., IEEE Trans. Image Process. 19, 3243 (2010).

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Title: Computation of Extremal Eigenvalues of High-Dimensional Lattice-Theoretic Tensors in Tensor-Train Format

Author(s): *Vesa Kaarnioja, *Aalto University*.

Initially studied due to their connection to the best rank-1 approximation problem of tensors, tensor eigenvalues have become an active topic of research in numerical multilinear algebra. Many spectral properties of matrices have been generalized to tensors in recent years, including generalizations of the power and shifted power method for the solution of tensor eigenvalues. However, the solution schemes for tensor eigenvalues are still subject to the so-called curse of dimensionality associated with applications involving tensors. In this talk, we propose implementations of the symmetric higher-order power method (S-HOPM [1]) and the generalized eigenproblem adaptive power method (GEAP [2]) in tensor-train format, which drastically lessens the computational complexity associated with these algorithms. As an application, we consider eigenvalue problems associated with the class of lattice-theoretic meet and join tensors, which may be regarded as multidimensional extensions of classically studied meet and join matrices such as GCD and LCM matrices, respectively. Meet tensors are shown to have an explicit low-rank tensor-train decomposition with sparse tensor-train cores with respect to the dimension. Moreover, this representation is independent of tensor order, which eliminates the curse of dimensionality from the numerical analysis of these objects and makes the solution of tensor eigenvalue problems tractable with increasing dimensionality and order. For join tensors, it is shown that a tensor-train decomposition with an a priori known TT-rank exists under general assumptions and this decomposition can be constructed numerically by using TT-cross approximation. Numerical experiments are used to assess the sharpness of existing theoretical estimates for the eigenvalues of meet and join tensors. [1] E. Kofidis and P. A. Regalia. On the Best Rank-1 Approximation of Higher-Order Supersymmetric Tensors. SIAM J. Matrix Anal. Appl. 23(3) (2002), pp. 863-884. [2] T. G. Kolda and J. R. Mayo. An Adaptive Shifted Power Method for Computing Generalized Tensor Eigenpairs. SIAM J. Matrix Anal. Appl. 35(4) (2014), pp. 1563-1581.

14th U.S. National Congress on Computational Mechanics
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Title: Fatigue Life Prediction for Critical Microstructures in AM Metals

Author(s): *Orion Kafka, Cheng Yu, Wing Kam Liu, *Northwestern University*.

In the ongoing effort to produce loadbearing or functional parts for mission-critical applications with AM materials, quantification and prediction of material behavior is an important factor. The ability to produce robust designs, optimize build conditions, assess the product, and finally approve for use these kinds of parts all depend upon understanding the properties, including the mechanical response, of the system. In general, there is a limited understanding of the material that results from the metal AM process, particularly when subjected to cyclic load conditions. Thus, this talk will present our work towards codifying critical microstructures for fatigue nucleation in AM materials using experiments and simulations. The experiments were conducted at the Advanced Photon Source at Argonne National Laboratory. Experiments include imaging and in-situ loading with x-ray CT, and crystallographic measurements with 3D micro-diffraction. These experiments provide initial conditions and validation data to a series of simulations based on imaged and image-inspired synthetic geometries. Such inputs can be used to probe the impact of competing factors such as void geometry and proximity, local crystallography, and surface effects on fatigue nucleation life. These parametric studies will be enabled by a concurrently developed reduced order model, derived from the self-consistent clustering analysis (SCA) method [1]. Simply, SCA reduces the number of operational degrees of freedom by solving for the material response of clusters of material points, wherein the properties are assumed to evolve uniformly, with similar mechanical response. The method described in [1] is modified so that a crystal plasticity law can be applied. This dramatically reduces the computational cost associated with determining fatigue incubation life, which is achieved through a Fatemi-Socie fatigue indicating parameter. This allows for accurate, direct assessment of relatively large features, such as clusters of voids caused by lack of fusion or boiling during a build. These simulations of potential worst-case configurations may help guide design and manufacturing of AM materials and parts. [1] Liu Z, Bessa M, Liu W (2016a) Self-consistent clustering analysis: An efficient multi-scale scheme for inelastic heterogeneous materials. Computer methods in applied mechanics and engineering 306:319–341.

14th U.S. National Congress on Computational Mechanics
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Title: Application of Fourier and Wavelet Methods to an Experimental Tumbling Mill Using 3D Particle Tracking Data

Author(s): *Daramy Kallon, *University of Johannesburg*; Indresan Govender, *UKZN*; Aubrey Mainza, *UCT*.

Fourier and wavelet methods are applied to data derived from Positron Emission Particle Tracking (PEPT) experiments conducted at the iThemba LABS outside Cape Town in South Africa. The methods are applied as an aid in developing a computational procedure for determining the value of the circulation rates of the charge found in typical industrial tumbling mills. The circulation rate values are obtained as fundamental harmonics from power spectral plots using Fourier analysis. The wavelet method is applied to identify and remove noise from the data in order to improve on the computationally determined value of the circulation rate. For the analysis presented herein, parameters are obtained directly from the flow dynamics of the PEPT tracer particle. Key words: Fourier and Wavelet methods, Circulation rates, Power draw Summary of Presentation Introduction – circulation rates of charge in tumbling mills Fourier and Wavelet Methods - Mathematical Application in Computational Mechanics The experimental approach Applying Fourier analysis to tumbling mill – using data from PEPT Applying Wavelet analysis to tumbling mill – using data from PEPT Results and discussions Conclusion Contribution to the field of Computational Methods in Image Analysis An investigation was conducted into the causes of the failure of the Fourier scheme developed for the computational determination of the value of the circulation rate of tumbling charge using data derived from PEPT experiments. It was observed that the main cause was the occurrence of high frequency components in the signal generated from the reconstructed data. These high frequency components effect as noise during data acquisition or pre-processing of the data. This paper contributes to the development of a better computational method for analyzing data obtained from PEPT, a technique derived from medical imaging procedures that is now being applied to some aspects of engineering.

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Title: Modeling Dynamic Shear Rupture at Weak Interfaces: In Quest of High Resolution and Precision

Author(s): *David Kammer, *Cornell University*.

Numerical modeling of shear ruptures at weak interfaces has, due to its great importance to structural engineering and geophysics, a long-standing history with significant progress. Various approaches including the finite-difference method, the finite-element method, and the spectral boundary integral method in combination with failure models based on cohesive elements and traction-at-split-nodes techniques have been applied for a large variety of applications. In this work, we focus on refining these methods to develop precise numerical models of high resolution that have the capability of providing quantitative prediction for dynamic shear crack propagation. We discuss factors that affect the numerical results and their usefulness for studying the underlying mechanisms of dynamic shear failure. These high-resolution numerical results are particularly valuable in combination with experimental observations. While the experimental measurement quality of dynamic shear cracks has significantly increased over the past decade and new quantities could be accessed, these observations still rely on a limited number of point measurements. For instance, measuring the tractions along the interface is essential to the development of accurate constitutive laws for friction and adhesion but impossible with strain gages that are glued at some finite distance from the interface. Extrapolation of measured stresses to estimate the interface tractions is challenging due to the highly non-linear character of the stress field around a non-steady dynamic shear rupture. The numerical models developed in this work, however, provide means to overcome this challenge. We show that many aspects of dynamic shear cracks, such as crack tip stress radiation, propagation speed, and crack arrest, can be quantitatively predicted by these numerical simulations and thus provide complementary insight into the fundamental mechanics of shear failure of weak interfaces and are key to establishing relevant constitutive interface laws. In addition, the area of relevance for various interface properties can be determined by comparing simulations and experimental observations under different conditions (e.g., the effect of the dynamic shear stress drop at the interface on the measured shear stress at a given distance from the interface depends significantly on the rupture speed).

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Title: Development and Validation of FSI Analysis System Considering Active Control

Author(s): *Shigeki Kaneko, Giwon Hong, Naoto Mitsume, Tomonori Yamada, Shinobu Yoshimura, *The University of Tokyo*.

Fluid-Structure Interaction (FSI) is an interdependent phenomenon between fluid and structure that affects their dynamic behaviors. The control of FSI is important in engineering because FSI often influences the structural integrity and lifetime of structures. Here, control methods are classified into active control and passive one. Generally, active control needs high cost because it requires external resources but can achieve more detailed control. Therefore, we focus on the former in this study. We use a simulation based study because it cuts the cost and time of experiments and suitable for parametric studies. Although there have been many simulation based studies about the control of FSI, fluid or structure is treated as simple models. There is little research which performs both fluid and structural analyses strictly and treats interaction conditions on the coupling interface precisely. In order to make it possible to treat more various FSI problems, we propose a new method in this paper. It is FSI analysis considering active control, which is established by integrating FSI analysis by partitioned iterative method and an algorithm of active control. Partitioned iterative method is one of the efficient and robust FSI analysis algorithms and we have analyzed complicated FSI problem by partitioned iterative method [1]. After we propose and implement FSI analysis considering active control, we analyze the two-dimensional vortex induced vibration problem of an elastically mounted cylinder, which is a famous benchmark problem. We evaluate the effect of active control by calculating the reduction of the amplitude of vibration. Comparing the effect with that of the existing numerical study [2], which was performed by Mehmood et al. on the same condition, we validated that the effect of active control appears properly. [1] T. Yamada et al. “Parallel partitioned coupling analysis system for large-scale incompressible viscous fluid structure interaction problems.” Computers&Fluids 141 (2016):259-268 [2] A. Mehmood et al. “Linear and nonlinear active feedback controls for vortex-induced vibrations of circular cylinders.” Journal of Vibration and control 20.8 (2014):1137-1147

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Title: Integrated Topology Optimization of Multi-Component Structures Considering Interface Behaviors

Author(s): Pai Liu, *Zhan Kang, *Dalian University of Technology*.

This paper presents a level set-based integrated topology optimization method for simultaneous optimization of the component layouts and the host structure topology of multi-component structures. We first propose a method to account for the behavior of the interconnect interface between the components and the host material. Here we treat the interconnect interface with the cohesive zone model. A conforming mesh in conjunction with the interface elements are employed to discretize the evolving structure while accounting for the strong discontinuity of displacement field across the interface. We also suggest a multi-material level set model to give clear representation of structural boundaries and the interconnect interface. An objective function that contains the work dissipated by the traction on the interconnect interface is considered and the evolution velocities of the level set functions are treated as the design variables. The sensitivities are derived with the adjoint method and the design variables are obtained with the MMA optimizer, which makes it easier to handle multiple constraints in level set based optimization problems. The design is updated via the Hamilton-Jacobi equation with the velocity design variables as inputs. Re-initialization is performed to preserve the signed distance property of the level set functions. Numerical examples are given to illustrate the validity and applicability of the proposed method.

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Title: Characterization of Near-Surface Road Cavity Using an Elastic Wave Full-Waveform Inversion Method

Author(s): Boyoung Kim, Seungwook Youn, *Jun Won Kang, *Hongik University, Korea*; Seong-Hoon Kee, *Dong-A University, Korea*; Haesang Jeong, *Korea Infrastructure Safety & Technology Corporation, Korea*.

This paper presents the characterization of near-surface road cavities using ground velocities measured on the surface of asphalt pavements due to impact loads. The characterization is performed by using a two-dimensional elastic wave full-waveform inversion (FWI) method, which attempts to utilize real data to estimate the location, size, and depth of the cavities under road pavements. To simulate elastic waves and satisfy the far-field radiation condition numerically, perfectly matched layer (PML) is introduced as wave-absorbing boundary for a finite computational domain of interest where the elastic moduli are sought to be reconstructed. The FWI method is implemented based on a partial-differential-equations-constrained optimization framework, which seeks the optimal values of elastic moduli of the PML-truncated domain while minimizing Lagrangian functional. The Lagrangian consists of a least-squares objective functional and regularization terms, augmented by the weak imposition of PML-endowed elastic wave equations via Lagrange multipliers. The spatial distribution of elastic moduli within the PML-truncated domain are reconstructed by solving iteratively the state, adjoint, and control problems which result from the stationarity conditions of the Lagrangian. Two asphalt pavement sites are considered for the characterization of cavities using the FWI method. The cavities with sizes of several meters and located at less than 5 meters from the surface have been successfully reconstructed using horizontal and vertical ground velocities measured on the pavement surface. The results of the ground cavity reconstruction as well as the details of impact loads, sensor layout, and response superposition technique for the two-dimensional FWI analysis are presented. References [1] J. W. Kang and L. F. Kallivokas, The inverse medium problem in heterogeneous PML-truncated domains using scalar probing waves. Computer Methods in Applied Mechanics and Engineering, 2011, 200, pp. 265-283. [2] A. Fathi, L. F. Kallivokas, and B. Poursartip, Full-waveform inversion in three-dimensional PML-truncated elastic media, Computer Methods in Applied Mechanics and Engineering, 2015, 296, pp. 39-72.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Dredging Induced Failure Mechanisms of Subaqueous Slopes– An Investigation with Coupled CFD-DEM

Author(s): *Manuela Kanitz, Jürgen Grabe, *TUHH*.

Shallow offshore structures like gravity foundations for offshore wind turbines can rarely be placed on top of the seabed as the weak top soil has to be excavated to place the structure on more stable ground. Steep but stable slopes of the resulting pit meets both economic and ecologic interest as it reduces the disturbance of the marine fauna and minimizes the material movement. Thereby, the dredging initiates a failure of the subaqueous slopes resulting in different slope angles. As the failure mechanisms of a subaqueous slope are barely investigated, relatively small final slope angles are set to guarantee a stable subaqueous slope during the construction. Nevertheless, small-scale experiments show that during dredging higher slope angles than the critical angle can be reached. Effects of dilatancy and contractancy in the soil bed and their influence on pore water pressure changes are crucial for the investigation of failure mechanisms in subaqueous slopes as the constant shearing of the sand bed triggers periodical changes between liquefaction and hardening. To include these effects into numerical simulations, a coupled Euler-Lagrange approach, namely the combination of Computational Fluid Dynamics (CFD) and the Discrete Element Method (DEM), is used. In these simulations, the liquid phase, e.g. the water, is considered as a continuum and the solid phase, e.g. the soil, is represented with particles. Hence, it is possible to compute the particle-particle- as well as the fluid-particle-interactions. The calculations are carried out with the open source software package CFDEMcoupling®, which combines the discrete element code LIGGGHTS® with CFD solvers based on OpenFOAM®. The dredging induced disturbance of subaqueous slopes will be investigated in model tests using glass beads in order to validate the results of the simulations using CFD-DEM. Afterwards, numerical investigations on sand will be carried out, whereas the soil grains are idealized by spherical particles of different diameters. In order to consider effects of dilatancy and contractancy in the soil bed, different relative densities are investigated.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Large-Scale All-Electron Density Functional Theory Calculations Using an Enriched Finite Element Basis

Author(s): *Bikash Kanungo, Vikram Gavini, *University of Michigan*.

Typically, in a DFT calculation, to afford both accuracy and computational efficiency, the effect of the core electrons and the nuclear potential is modeled into a smooth effective potential, called the pseudopotenial. Although successful in predicting various properties over a wide range of materials, they tend to oversimplify the treatment of the core electrons as chemically inert and bear inaccurate results for several material properties like the bulk properties in transition metals, phase transitions in systems under high pressure, spectroscopic properties in heavy metals, band-gaps and excited state properties, to name a few. This calls for an accurate all-electron DFT method which can dispense with the pseudopotentials without incurring too much computational cost. We achieve the above by using an enriched finite element basis wherein the classical finite element basis is augmented with compactly supported atom-centered numerical basis functions obtained from the solution of the Kohn-Sham (KS) problem for single atoms, so as to efficiently capture the electronic fields near nuclei as well as preserve the completeness of the basis. These augmenting functions are termed as enrichment functions. The compact support for the enrichment functions is obtained by using smooth cutoff functions, which enhances the conditioning and maintains the locality of the resultant basis. Additionally, the integrals featuring in the KS problem discretized in the enriched finite element basis are evaluated using an adaptive quadrature grid constructed based on the characteristics of the enrichment functions. We also propose an efficient inversion of the overlap matrix based on block-wise matrix inversion and the use of special reduced-order quadrature rules, thereby transforming the discrete KS problem to a standard eigenvalue problem. Finally, we employ a Chebyshev polynomial based filtering technique to evaluate the occupied KS eigenspectrum. The accuracy and efficiency of the method is assessed against semiconducting (Si) and heavy-metallic (Au) systems of various sizes, with the largest system containing 8694 electrons. We obtain accuracies in ground-state energies that are within ~1mHa when compared to both classical finite element as well as gaussian basis. In terms of computational efficiency, we achieve a 50–300 and a ~8 fold reduction in the overall computational time when compared to classical finite element and gaussian basis, respectively. We also observe good parallel scalability up to 384 processors for a benchmark 280-atom silicon nano-cluster. References: B. Kanungo and V. Gavini, Physical Review B 95, 035112 (2017).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Practical Approach to Curving Meshes for Realistic Geometries

Author(s): *Steve Karman, *Pointwise, Inc.*.

Linear element meshes for complex geometries are elevated to high order and curved using a multi-step process. The linear meshes are first elevated to high order by introducing new edge, face and internal nodes, increasing the polynomial degree to P2, P3 or P4. Then the new surface nodes are projected onto the true geometry using discrete and/or CAD geometry. These surface node perturbations are then used to position the interior nodes to ensure a valid, high quality mesh results. This presentation documents enhancements to the method presented in AIAA-2016-3178.1 The most difficult aspect of high order mesh curving is the requirement to have valid elements in clustered meshes near curved boundaries. The projection of surface nodes can produce element inversion and result in negative Jacobians. Several techniques are available to position the interior nodes. The simplest method propagates the surface perturbations through a direct transfer to nearest neighbor nodes using the mesh connectivity. This method is not guaranteed to produce valid meshes. The next method solves the Winslow elliptic smoothing equations in a finite volume formulation or finite element formulation. The unperturbed mesh serves as the computational mesh for solving the Winslow equations. In the finite volume formulation the unperturbed high order elements are subdivided into linear elements and the Winslow equations are solved on the linear elements. In the finite element formulation the Winslow equations are solved directly on the unperturbed high order elements. Winslow elliptic methods are inherently smooth. The implementation imposes the character of the unperturbed mesh onto the physical mesh, so the grid clustering is preserved. Initial testing has produced valid meshes in most cases. The third method, and the one that finally ensures mesh quality and validity, uses a Weighted Condition Number based optimization scheme. In the WCN method the shape of the unperturbed, linear sub-elements is imposed on the final mesh. Any boundary perturbation, especially in viscous regions of curved geometry, is transferred through the mesh by optimizing the node position to achieve the original unperturbed shapes. The resulting mesh is only curved near curved boundaries. The majority of the interior mesh edges remain straight. Several realistic three-dimensional meshes are presented including AIAA DPW 6, AIAA High-Lift PW 3 and BANC-III landing gear. Reference: [1] Karman, S. L., Erwin, J. Taylor, Glasby, Ryan S., Stefanski, Douglas L., “High-Order Mesh Curving Using WCN Mesh Optimization”, AIAA-2016-3178, AIAA Aviation 2016, Washington, DC, June 2016.

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14th U.S. National Congress on Computational Mechanics
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Title: 2D and 3D Finite Element Analysis for Tsunami Waves

Author(s): *Kazuo Kashiyama, Guoming Ling, *Chuo University*; Junichi Matsumoto, *AIST*.

Tsunamis kill many human beings and seriously hinder economic activities, such as the tsunami caused by the Great East Japan Earthquake in 2011. It is very important to develop useful modeling and simulation methods for tsunami waves in order to perform the planning and design for community development and the prevention of disasters. In this presentation, the modeling and simulation methods are presented for tsunami waves. The stabilized finite element methods based on Lagrangian approaches are employed for tsunami simulations. In order to realize an efficient tsunami simulation, a combination method using 2D and 3D models is presented. The shallow water equation and Boussinesq equation are employed for the governing equation for 2D simulation. The Navier-Stokes equation is employed for the governing equation for 3D simulation. The VOF method and phase-field method are employed for the 3D simulation. The present modeling and simulation methods are shown to be useful tools to achieve high quality in large scale tsunami simulations.

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14th U.S. National Congress on Computational Mechanics
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Title: Representative Elementary Volume Modeling of Geopolymer Composites

Author(s): *Amrita Kataruka, Waltraud Kriven, Ange Therese-Akono, *University of Illinois at Urbana-Champaign, USA*; Erman Guleryuz, Seid Koric, *National Center for Supercomputing Applications, USA*.

The research objective is to elucidate the microstructure-strength relationships in geopolymer composites. Geopolymer is an inorganic polymeric material, which consists primarily of alumina, silica and alkali metal oxides. Geopolymer composites exhibit excellent adhesive, thermal, and chemical properties making them relevant in a diverse range of applications such as fire resistant materials, environment-friendly binders, composites for infrastructure repair/strengthening, radioactive waste containment, furnace molds etc. Despite the surge in interest in geopolymeric materials, a mechanistic study of the correlation between composition and performance is still missing. In turn, the lack of advanced theoretical tools to predict the mechanical performance is a recognized obstacle to the widespread adoption of geopolymer-based materials in standards and building codes. Therefore, our goal is to formulate a periodic micro-field approach to assess the effective elastic moduli and strength properties as a function of the microstructure and the individual phases. We articulate a four-level thought-model for geopolymer composites. At the elementary level- the molecular scale, exists the basic unit, which consists of [SiO4] and [AlO4] tetrahedral surrounded by alkali monovalent cations. At the microscopic level, exists the geopolymer precursor which is an amorphous aluminosilicate gel. Due to the nano-granular and nano-porous nature of the geopolymer matrix, the plastic yield criterion is pressure-sensitive. At the meso-scale, four constituents can be identified: the matrix, micro-pores, inclusions and unreacted phases. At the macroscopic scale, the material is homogeneous. Numerical simulations are carried out to connect the meso and macroscopic scales. A numerical representative elementary model is defined where the filler is modeled as inclusions embedded in a homogeneous matrix. Both tensile and compression tests are simulated and the resulting effective properties and failure mechanisms are computed. The finite element homogenization scheme is validated using independent experiments on particle-reinforced and fiber-reinforced potassium-based geopolymer composites. The influence on the effective response of intrinsic factors such as filler content, filler aspect ratio, filler angularity, filler spatial distribution, interface bonding, and processing procedure is studied. The effective strength increases as the filler volume fraction and the filler aspect ratio increase. Furthermore, stronger bonding at the interface and controlled synthesis methods result in enhanced strength characteristics. This novel bottom-up multi-scale modeling framework enables the virtual mechanical testing of geopolymer-based composites.

14th U.S. National Congress on Computational Mechanics
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Title: Development of Multi-Scale MPF Topology Optimization to Maximize a Heat Conductivity Assuming a Metallic Crystalline Structure

Author(s): *Junji Kato, Toshiki Ichibangase, Shun Ogawa, Takashi Kyoya, *Tohoku University*; Tomohiro Takaki, *Kyoto Institute of Technology* .

The material design to obtain an optimal microstructure applying a numerical approach is receiving a lot of attention, especially in the field of advanced materials, such as special alloys and fiber reinforced polymers. However, the geometry of microstructure of alloys shows complex crystalline structure, which the conventional topology optimization is unsuitable to represent. For this reason, the present study challenges to develop topology optimization scheme for crystalline metals applying the Multi-Phase Field (MPF) method. The objective is to maximize the heat conductivity of a macrostructure consisting of dual-phase crystalline metal with respect to a prescribed material volume. In this context, multi-scale analysis must be considered to represent the hierarchical and mechanical relationships between different scales and these relationships also must be affected to the optimization algorithms. This challenging work should be of great value in the field of material science and material design and its versatile framework is introduced in this research. The proposed method is examined by a series of numerical examples and eventually verified that it can provide a reliable optimal design for crystalline metals to maximize the heat conductivity of a macrostructure.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Coupled Overset Mesh and Hybridizable Discontinuous Galerkin Algorithm for Dynamic ALE Formulations

Author(s): *Justin Kauffman, Jonathan Pitt, *Pennsylvania State University*.

Traditional overset mesh methods in a finite volume or finite difference context are not, generally, arbitrarily high-order accurate because to increase the approximation order the amount of overlap between meshes must increase [1]. This increasing amount of overlap requires a larger number of fringe cells, cells with a suitable donor, to be stored, and used for communication between meshes, in order to obtain high-order accurate solutions. Other overset methods that do not require any specific amount of overlap, like the discontinuous Galerkin (DG) Chimera scheme developed by Galbraith et. al. [2], have large numerical systems. These large systems are derived from duplication of degrees of freedom (DoFs) on element boundaries, and high-order approximations exacerbate this issue. In an overset context the numerical sys- tem becomes even larger because the system must contain all the meshes, and the coupling between the meshes. The coupled overset mesh and hybridizable discontinuous Galerkin (HDG) algorithm reduces the numerical system, and is arbitrarily high-order accurate for arbitrary overlap between meshes. The HDG method reduces the global numerical system through hybridization [3]. Hybridization allows for the formation of the Schur complement to be utilized to eliminate the local solution from numerical system, greatly reducing the system to just contain the global DoFs. After the global solution is obtained, the local solution for each cell can be obtained independently for each cell, which is ideal for parallel algorithms. The goal of this work is to simulate full-scale hydrodynamics problems. To achieve these simulations, the necessary building blocks must first be verified and validated. One such building block is the numerical formulation of dynamic Arbitrary Lagrangian-Eulerian (ALE) problems. Simulating these problems with a single mesh would result in either a poor quality mesh or remeshing the domain frequently. Simulating the problem via an overset method improves mesh quality, and there is no need for remeshing. Verification and validation are performed to demonstrate the applicability of the overset HDG algorithm. References [1] R. W. Noack, SUGGAR: a General Capability for Moving Body Overset Grid Assembly, 17th AIAA Computational Fluid Dynamics Conference (2005). [2] M. C. Galbraith, J. A. Benek, P. D. Orkwis, and M. G. Turner, A Discontinuous Galerkin Chimera Scheme, Computers & Fluids 98 (2014) 27–53. [3] N. Nguyen, J. Peraire, Hybridizable discontinuous Galerkin method for partial differential equations in continuum mechanics, Journal of Computational Physics 231 (2012) 5955–5988.

14th U.S. National Congress on Computational Mechanics
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Title: Constitutive and Computational Modelling with Fluid-Structure Interactions of Venous Tissues

Author(s): *Nayyan Kaul, Hsiao Ying Shadow Huang, *MAE, North Carolina State Uni.*.

Venous valve tissues, while used in vein reconstruction surgeries and bio prosthetic valves with moderate success, does not have extensive studies on their structure and modelling. Their inherent anisotropic, non-linear behavior combined with severe diseases inflicting the veins like chronic venous insufficiency warrants understanding the structure and material behavior of venous valve tissues. With the scant information on uniaxial and biaxial mechanical properties of jugular venous valve and wall tissue from any previous studies, the current focus of our study was to understand the material behavior by determining an established phenomenological strain energy based constitutive relation for the tissues. First, we used bovine veins to experimentally study the behavior of valve leaflet tissue and adjoining wall tissue (from proximal and distal end of the vein) under different biaxial testing protocols. Second, we looked at the behavior of numerical partial derivatives of strain energy to select a suitable functional form of strain energy for wall and valve tissue from the literature [1-3]. Using this strain energy descriptor, we determined Cauchy stress and compared it with experimental results under displacement controlled biaxial testing protocols to find material specific model parameters by Powell's method algorithm. We then implemented our selected constitutive models along with material specific model parameters using user defined material subroutines (UMAT) in a commercial FEM package ABAQUS with fluid-solid interactions (FSI) functionality. We observe the blood flow behavior differences around a bileaflet versus a trileaflet valve during opening/closing in the vein. Isolated and coupled effects from hemodynamic, hydrostatic, and hydrodynamic variations are studied based on the FSI simulations. Results indicated that whereas wall tissue strain energy can be explained using a polynomial nonlinear function, the valve tissue, due to higher nonlinearities, requires an exponential function. This study can prove helpful in primary stages of bio-prosthetic designs; replacement surgeries; can be of support to any future studies investigating structural models and to study valvular diseases by giving a way to understand material properties, and to form a continuum model required for numerical analyses and simulations. References: [1] Humphrey JD, Strumpf RK, Yin FCP. Journal of Biomechanical Engineering. 1990; 112(3):333-339. doi: 10.1115/1.2891193. [2] Humphrey JD, Strumpf RK, Yin FCP. Journal of Biomechanical Engineering. 1990; 112(3):340-346. doi: 10.1115/1.2891194. [3] May-Newman K, Yin FCP. Journal of Biomechanical Engineering. 1998; 120(1):38-47. doi: 10.1115/1.2834305.

14th U.S. National Congress on Computational Mechanics
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Title: Modeling and Simulation of the Dynamics of Soft Adhesion Mediated by Mobile Binders: 2D Variational Modeling

Author(s): *Dimitri Kaurin, Marino Arroyo, *LaCaN UPC, Spain*.

Abstract We re-examine a classical problem in soft-matter physics: the specific adhesion between deformable elastic objects, such as vesicles, mediated by mobile adhesion molecules. Physically and from a continuum perspective, the system can be understood as a membrane with bending rigidity, subject to a fixed tension by a loading device such as a micropipette, with mobile adhesion molecules. These molecules can diffuse and react by attaching with partners in a neighboring vesicle. The binding kinetics strongly depend on the distance to potential partners in the neighboring membrane. The unbinding kinetics depend on the force experienced by the binders. Moreover, bonds can exhibit different force dependent rates such as catch bonds or slip bonds (1). Such problems are well studied at equilibrium but the dynamics have been barely explored. Following seminal work (2), which identifies possible scenarios governing the dynamics of binding or unbinding, the system is treated as a biphasic problem with a sharp interface delimitating the bound and unbound regions of the vesicle. The force and distance dependent binding/unbinding kinetics are captured by coupling this large-scale model with a smaller-scale model relying on scale separation. We have formalize the problem in the framework of Onsager's variational principle (3), providing a systematic procedure to generate the governing coupled equations of the problem that capture the interplay between diffusion, reaction and mechanics and we examine this problem with numerical calculations. The emphasis here is made on the binding-unbinding dynamics, the influence of their conformation and the corresponding force-dependence of the unbinding rate of adhesion molecules. Bibliography [1] S. Rakshit, Y. Zhang, K. Manibog, O. Shafraz, and S. Sivasankar, "Ideal, catch, and slip bonds in cadherin adhesion," Proceedings of the National Academy of Sciences, vol. 109, no. 46, pp. 18815–18820, 2012. [2] P.-G. de Gennes, P.-H. Puech, and F. Brochard-Wyart, "Adhesion Induced by Mobile Stickers: A List of Scenarios," Langmuir, vol. 19, pp. 7112–7119, aug 2003. [3] M. Doi, "Onsagers variational principle in soft matter," Journal of Physics: Condensed Matter, vol. 23, no. 28, p. 284118, 2011.

14th U.S. National Congress on Computational Mechanics
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Title: Adaptive Simulation of Coastal and Hydraulic Fluid-Structure Interaction in the Proteus Toolkit

Author(s): *Chris Kees, Matthew Farthing, *US Army ERDC*; Manuel Quezada de Luna, *US Army ERDC/ORISE*; Alvin Zhang, Onkar Sahni, *RPI*; Tristan de Lataillade, Aggelos Dimakopoulos, *HR Wallingford, Ltd.*.

Engineering analysis of structures, vessels, and vehicles in complex, three-dimensional, multi-phase flows will soon be standard practice in coastal and hydraulic engineering due to integrated advances in high-performance computing, scalable parallel algorithms, and automated meshing. We will present recent development combining the Proteus toolkit for computational methods and simulation with the Parallel Unified Mesh Infrastructure (PUMI) to achieve simulation of floating solids under complex wave and current forcing. The approach is based on redistributing the boundary fitted geometry globally while simultaneously adapting the topology locally to achieve robust and accurate fluid-solid interaction dynamics. A key technology underpinning the methods are the stabilized finite element methods for incompressible free-surface flows, which generalize to higher-order and designed to minimize dependence on arbitrary parameters and mesh sensitivity while achieving qualitatively correct features such as mass/volume conservation and discrete maximum principles. These algorithms are combined in the open source Proteus toolkit in order to provide a framework for building parallel, adaptive applications for 3D coastal and hydraulic engineering analysis. Applications will be presented from a suite of verification and validation test under cooperative development led by the US Army Engineer Research and Development Center and HR Wallingford, Ltd.

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Title: Goal-Oriented Error Estimation and Adaptivity with the DPG Methodology

Author(s): *Brendan Keith, Ali Vaziri Astaneh, Socratis Petrides, Leszek Demkowicz, *UT Austin*.

The discontinuous Petrov-Galerkin (DPG) finite element methodology can be used to generate a wide variety of modern finite element methods which are naturally stable and possess a built-in a posteriori error estimator which can be used for adaptive mesh generation. We develop a number of goal-oriented error estimators for DPG by exploiting properties unique to the methodology and illustrate their utility in some example problems.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Sequential Convex Methods for Large-Scale Topology Optimization

Author(s): *Graeme Kennedy, *Georgia Institute of Technolog*.

Large-scale applications of topology optimization rely on both efficient algorithms and the efficient use of computational resources. While many authors have made significant progress on large-scale topology optimization methods applied to complex structural configurations, continuing progress will require new algorithmic advances. In this work, we describe a new sequential convex method that is designed for good performance on large-scale topology optimization problems. The proposed sequential convex method leverages the extensive algorithms and theory behind convex optimization. The compliance of a linear structure is convex when the stiffness matrix is an affine function of the design variables. However, most conventional topology optimization formulations are naturally non-convex. Density-based penalization methods break convexity by using stiffness matrix parametrizations that are a nonlinear function of the design variables. Alternative penalization strategies, such as concave penalty functions, introduce non-convexity directly in the objective function or constraints. Within this work, we solve non-convex combined multimaterial and topology compliance problems. To handle the multimaterial aspect of the problems, we build on recent developments in the field of Discrete Material Optimization (DMO). DMO techniques were developed as a generalization of multiphase design methods and have subsequently been applied to a broad range of problems including multimaterial optimization. In a departure from previous topology optimization techniques, we create a convex sub-problem at each iteration of the optimization algorithm by constructing a convex approximation of the penalized compliance. This approach is similar to the concave-convex procedure from the convex optimization literature. The proposed method does not make the overall optimization problem convex, but it is designed to leverage the extensive theory and methods available for convex optimization problems. In practice, the proposed algorithm can be implemented using any general purpose nonlinear optimizer to solve the convex sub-problems that arise at each iteration. However, better performance can be achieved when the optimizer exploits the convexity properties of the sub-problems. The performance of the proposed sequential convex method will be presented on a variety of problems, including a series of moderate-scale ground structure truss problems, 2D plane stress problems and large-scale 3D problems. These problems will illustrate the broad applicability of this class of sequential convex methods.

14th U.S. National Congress on Computational Mechanics
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Title: A Posteriori Mesh Quality Control in Probabilistic Bayesian Inversion

Author(s): *Pierre Kerfriden, Abhishek Kundu, Susanne Claus , *Cardiff University* .

The quality of finite element meshes used in probabilistic inverse problems can have a tremendous impact on the reliability of the results. In this work, we attempt to connect the field of adaptive methods for the accuracy of deterministic and forward probabilistic simulations and the field of Finite-Element based Bayesian inference. In particular, our target setting is that of exact inference, whereby complex posterior distributions are to be sampled using advanced Markov-Chain Monte-Carlo (MCMC) algorithms. Our proposal is for the mesh refinement to be performed in a goal-oriented manner. We assume that we are interested in a finite subset of quantities of interest (QoI) such as a combination of latent uncertain parameters and/or quantities to be drawn from the posteriori predictive distribution. Next, we evaluate the quality of an approximate inversion with respect to these quantities. This is done by running two chains in parallel: (i) the uncorrected approximate chain and (ii) an enhanced chain whereby the approximate likelihood function is corrected using an efficient deterministic error estimate, possibly augmented with probabilistic terms. One particularly interesting feature of the proposed approach is that no user-defined tolerance is required for the quality of the QoIs, as opposed to the deterministic error estimation setting. This is because our trust in the model, and therefore a good measure for our requirement in terms of accuracy, is fully encoded in the prior. We merely need to ensure that the finite element solver does not impact the posterior distributions of QoIs by a large amount. We will also propose a technique to control the error introduced by the MCMC sampler, and demonstrate the validity of the combined mesh and algorithmic quality control strategy.

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Title: Goal-Oriented Proper Generalized Decomposition with Error Estimation and Adaptivity

Author(s): *Kenan Kergrene, Serge Prudhomme, Marc Laforest, *Ecole Polytechnique Montréal*; Ludovic Chamoin, *Ecole Normale Supérieure de Paris-Saclay*.

The talk will deal with the development of a mathematical formulation aiming at constructing adaptive reduced-order models tailored for the approximation of quantities of interests. The main idea is to formulate a constrained minimization problem that includes inequalities on the error in the goal functionals so that the resulting model be capable of delivering enhanced predictions of the quantities of interest within some prescribed tolerances. The formulation will be applied to the so-called Proper Generalized Decomposition (a low-rank approximation) method. Such a paradigm represents a departure from classical goal-oriented approaches where the reduced model is first derived by minimization of the energy, or of the residual functional, and subsequently adapted via a greedy approach by controlling a posteriori error estimates measured in terms of quantities of interest using dual-based error estimates. Numerical examples will be presented in order to demonstrate the efficiency of the proposed approach.

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Title: Topology Optimization under Uncertainty via Non-Intrusive Polynomial Chaos Expansion

Author(s): *Vahid Keshavarzzadeh, *University of Illinois* ; Daniel Tortorelli, *University of Illinois*.

We present a systematic approach for topology optimization under uncertainty that integrates non-intrusive polynomial chaos expansion with design sensitivity analysis for reliability-based and robust topology optimization. Uncertainty is introduced in loading and in geometry to address the manufacturing variability. The manufacturing variability is modeled via a thresholding technique in which the threshold field is represented by a reduced dimensional random field. Response metrics such as compliance and volume are characterized as polynomial chaos expansions of the underlying uncertain parameters thus allowing accurate and efficient estimation of statistical moments, failure probabilities and their sensitivities. The number of simulations is reduced for linear structures under loading uncertainty by means of superposition. Efficiency of the non-intrusive polynomial chaos approach is highlighted by comparison with the Monte Carlo method in terms of the number of simulations. To demonstrate the effect of uncertainty, optimized designs that consider uncertainty are compared to those that do not. Comparisons of polynomial chaos expansion to existing analytical methods on a benchmark numerical example are also provided for reliability-based and worst case designs.

14th U.S. National Congress on Computational Mechanics
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Title: Energy Renormalization Approach to Coarse-Graining of Polymer Dynamics

Author(s): *Sinan Keten, Jake Song, Wenjie Xia, *Northwestern University*; Cheol Jeong, Fred Phelan, Jack Douglas, *NIST*; David Hsu, *Wheaton College*.

A major challenge in soft matter science is the bottom-up prediction of the temperature-dependent behavior of amorphous glass-forming (GF) polymers. Coarse-grained (CG) models derived from atomistic simulation data offer chemical specificity and access to relevant time- scales, but exhibit faster dynamics due to their reduced degrees of freedom. Based on the common notion of a temperature-dependent activation energy in glass formation theories, we find that renormalizing the CG cohesive energy parameters as a sigmoidal function of temperature allows accurate prediction of atomistic polymer dynamics over the Arrhenius, the non-Arrhenius, and the localized elastic regimes. We establish a rigorous approach to enthalpically compensate for the altered configurational entropy and cooperatively rearranging regions (CRRs) in CG modeling. This represents critical progress for building temperature- transferable CG models that predict key properties of a GF polymer. The unique role that cohesive interactions play on GF characteristics as highlighted in this work reveals new opportunities for the tailored design of GF polymer materials.

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Title: Predictive Modeling of Wavelet Coefficients for Physical Processes

Author(s): *Mohammad Khalil, Jina Lee, Maher Salloum, *Sandia National Laboratories*.

Simulation technology has become an integral and essential part of modeling many physical systems for various purposes including (a) gaining insight into the behavior of such systems, (b) predicting system behavior for decision-making purposes, and (c) calibrating models using available field observations. Large-scale simulations are becoming ubiquitous in science and engineering due to the rapidly-increasing complexity of problem domains leading to large and complex numerical models. In that context, the argument that cheap simulations may replace unmanageable, expensive, and/or risky experiments of real physical systems starts to lose traction since large-scale simulations are enabled by exascale computing and are thus quite expensive. To that extent, we aim to construct low-dimensional data-driven models that strive to capture the high-dimensional outputs from large-scale physics-based model simulations. These data-driven models are calibrated using high-dimensional data from large-scale simulations and subsequently provide accurate yet cheap predictions of model outputs. Compressed Sensing (CS) will be used for dimensionality reduction, mapping the high-dimensional simulation outputs to an alternative low-dimensional function space. The resulting wavelet coefficients are subsequently modeled using autoregressive-moving-average (ARMA) time series models and the Kalman filter is used to tackle the inverse problem of ARMA model calibration and subsequent predictions of wavelet coefficients. The predicted wavelet coefficients are used to reconstruct predicted system response, thereby replacing costly large-scale simulations. The ARMA modeling and forecasting is carried out at the low-dimensional setting due to the decreased required complexity and ability of CS to extract features of interest while filtering unwanted noise in the simulation outputs. We exercise the proposed methodology on two examples involving unstructured-mesh data. The first example involves the transient response of the two-dimensional heat equation on a square domain with randomly chosen holes (for added heterogeneity). For this example, the resulting wavelet coefficients follow a smooth and decaying time evolution with the ability to accurately forecast two time-instances of the wavelet coefficients instance for every 5 available time instances. The second involves larger data sets describing three-dimensional turbulent flows obtained from large-scale parallel simulations. For this second example the wavelet coefficients have oscillatory tendencies and the proposed methodology is able to accurately forecast one time-instance of the wavelet coefficients instance for every 4 available time instances. In both examples, the compound normalized root-mean-square error due to dimensionality reduction and forecasting falls in an acceptable range of 5 to 10%.

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Title: Turbulent Boiling Multiphase Flows using Variational Multiscale FEM

Author(s): *Mehdi Khalloufi, Youssef Mesri, Rudy Valette, Elisabeth Massoni, Elie Hachem, *Mines ParisTech*.

We propose in this work an adaptive variational multiscale FEM framework to solve two phase compressible-incompressible fluid flows undergoing phase change. In spite of the maturity and the popularity of numerical formulations, several involved mechanisms are still not well resolved. For complicated liquid-vapor dynamics, phase change, surface tension, interface mass transfer and discontinuous material properties have to be considered. We derive a unified compressible-incompressible variational multiscale formulation [1] designed to handle the abrupt changes at the interface and large density and viscosity ratio. An implicit implementation of the surface tension in the context of the Continuum Surface Force is proposed [2]. We propose a robust interface capturing method to follow efficiently and accurately the interfaces, but also to consider carefully high jump of different materials properties. It is based on the use of a modified conservative level set method that enables a direct localized level set re-initialization. We show that anisotropic mesh adaptation, combined with an a posteriori error estimator [3], yields an accurate 3D modeling framework for turbulent multiphase flows with phase change. We propose several time-dependent challenging benchmarks and compare the results with the literature and experimental data of boiling multiphase flows. References: [1] E. Hachem, M. Khalloufi, J. Bruchon, R. Valette, Y. Mesri, Unified adaptive Variational MultiScale method for two phase compressible-–incompressible flows, Comp. Meth. Appl. Mech. Engrg, 308:238-255, 2016, [2] M. Khalloufi, Y. Mesri, R. Valette, E. Massoni, E. Hachem, High fidelity anisotropic adaptive variational multiscale method for multiphase flows with surface tension, Comp. Meth. Appl. Mech. Engrg, Volume 307:44-67,2016, [3] T. Coupez and E. Hachem, Solution of high-Reynolds incompressible flow with stabilized finite element and adaptive anisotropic meshing, Comp. Meth. Appl. Mech. Engrg, 267:65-85, 2013

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Title: Modeling of Packing Processes for Ellipsoidal Particles of Arbitrary Size

Author(s): *Elham Kheradmand Nezhad, Leince Remson Elysée, Serge Prudhomme, Marc Laforest, *Ecole Polytechnique-Montréal*; Varvara Roubtsova, Mohamed Chekired, *IREQ Hydro-Québec*.

The subject of the talk will be concerned with the modeling and simulation of dense packing processes for ellipsoidal particles of arbitrary size. The goal is primarily to assemble samples of grains in order to numerically predict liquefaction, the phenomenon by which water-saturated soil temporarily loses strength due to dynamical loading such as in earthquakes. Soil liquefaction can have dramatic consequences, e.g. collapse of entire buildings or destruction of dams and retaining structures. These simulations are usually performed using spherical particles. However, this simple description of the particles fails in general to provide accurate predictions of the behavior of actual grains of sand, one of the reasons being that contact forces are incorrectly evaluated. The packing process consists in randomly dropping ellipsoids in a container and applying unidirectional vibrations to the container to achieve dense packing, until a desired height is achieved and particle sit in a stable position. Interactions between particles are simulated in this work using the Discrete Element Method. Numerical examples will be presented and results will be compared to spherical particles simulations in order to demonstrate the efficiency of the proposed approach.

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Title: Optimal Sensitivity of Nanowire Field-Effect Troponin Sensors

Author(s): *Amirreza Khodadadian, *Vienna University of technolog*; Clemens Heitzinger, *Vienna University of technology*; Kiarash Hosseini, Reza Kalantarinejad, Marjan Hedayati, Ali Manzour-ol-Ajdad, *Shezan Research and Innovation Centre*.

We have developed the simulation capability to design nanowire field-effect biosensors for the detection of proteins including the capability to include certain types of noise and fluctuations. The basic model equation is the stochastic drift-diffusion-Poisson system augmented by auxiliary calculations [1]. The application considered here is the detection of cardiac troponin, which is released after the heart muscle has been damaged, e.g., during a myocardial infarction. Cardiac troponin levels are normally so low that they cannot be detected with most blood tests. Despite many advantages of the currently used test, it usually takes four hours, which is too long in urgent-care scenarios. Reliable, sensitive, and fast troponin tests would make it possible to determine with certainty if a heart attack has occurred and thus to use the correct treatment. For modeling the electrostatic response, the partial charges of the known structure of troponin (PDB code 1MXL) as a function of pH value have been used. The random association and dissociation of the target molecules to and from the receptors at the sensor gives rise to biological noise. We therefore use the stochastic drift-diffusion-Poisson system [2] to model charge transport in the sensor, the stochastic Poisson-Boltzmann equation to model the electrolyte, and a reaction equation to model the association-dissociation processes at the surface. We present numerical results for the optimization of the sensitivity of the sensor for three different, important concentration regimes. The stochastic drift-diffusion-Poisson system also serves as a leading example for the development of optimal numerical algorithms for systems of stochastic PDE. References: [1] Amirreza Khodadadian, Kiarash Hosseini, Ali Manzour ol Ajdad, Marjan Hedayati, Reza Kalan- tarinjead, and Clemens Heitzinger. Optimal design of nanowire field-effect troponin sensors. 2017. Submitted for publication. [2] Leila Taghizadeh, Amirreza Khodadadian, and Clemens Heitzinger. The optimal multilevel Monte- Carlo approximation of the stochastic drift-diffusion-Poisson system. Computer Methods in Applied Mechanics and Engineering (CMAME). At press.

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Title: A Plate Model for Multilayer Graphene Sheets and Its Application to Analyzing Wrinkle Structure

Author(s): *Moonhong Kim, Seyoung Im, *KAIST*.

Multilayer graphene sheets (MLGSs) are stacks of single-layer graphene, which has exceptionally high stiffness and strength. They have distinct optical, electronical, thermal and mechanical properties. Owing to their superior features, there are various applications of MLGSs, such as composites, sensors, semiconductors, optomechanical devices and flexible devices. It is necessary to predict the mechanical behavior of MLGSs, from the atomistic scale to the continuum scale, when designing MLGS-based applications. A promising cost-efficient method by which to analyze MLGSs is a fully continuum-based method such as FEM. In this study, an equivalent continuum model for MLGSs and its structural element are developed to analyze the deformation behavior of MLGSs. Hyperelastic material models are introduced for the MLGS continuum model by examining the atomistic structures of MLGSs and obtaining their mechanical properties by means of molecular statics simulations. The MLGS plate model, a structural model, is developed by assuming the kinematics of the MLGS continuum model. Its plate element, termed the MLGS plate element, is implemented using FEM with the aid of the corotational formulation. The two numerical examples show that the proposed MLGS plate model feasibly represents the deformation behavior of MLGSs under elastic deformation from the atomic scale to the structural scale. Finally, wrinkle structures of MLGSs are studied by using the MLGS plate element with various scales and numbers of layers.

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Title: Topology Optimization of a Crash Box Considering Time-Dependent Crash and Nonlinear Plastic Behaviors Using Equivalent Static Loadings

Author(s): *Cheol Kim, Mohammadmahdi Davoudi, *Kyungpook National University*.

The securement of crashworthiness is an important goal in the design of energy absorbing structural components especially such as thin-walled structures. One of the important automotive structural parts is the thin-walled crash box which is placed behind the rear and front bumpers to protect passengers from the crash impact. The structure deforms at the time of a frontal or a rear crash and absorbs the energy of the crash impact before the extensive interior collapse of a vehicle. Therefore, it is required to ensure high energy absorption with a least amount of material. In this study, advanced impact analysis and the topology optimization with the modified the equivalent static loads (ESLs) have been newly developed and applied for the highly nonlinear axial crushing and folded plastic buckling problem of thin-walled crash-box structure. ESLs are defined as the equivalently linear static loads that generate the same displacement fields from linear static analysis as those from nonlinear dynamic analysis at each specified time step. The prior step to generate accurate ESLs is to incorporate the dynamic characteristics such as inertia and damping effects (i.e., forces) in the early stage of ESLs resulted from the nonlinear finite element crash analyses, and this process consequently transforms a dynamic crushing problem to a static one. A novel approach that is highlighted and adopted in this research is the application of the fine incremental time steps to calculate accurate ESLs from the extremely nonlinear fully crushing behaviors during the axial crash. The fine incremental step can cause an accurate linearization of the crushing plastic behaviors and is of extreme importance in capturing the nonlinear dynamic behavior of thin-walled structures to be applied for a topology optimization. An improved topology optimization for nonlinear dynamic responses is suggested with the ESLs. First of all, nonlinear dynamic analysis is performed and then ESLs are generated, and linear static topology optimization is performed with the obtained ESLs. This procedure repeats until the satisfaction of a specified convergence criterion. In this study, it is focused on applying the shell elements to capture the behaviors of thin-walled structures by means of plastic hinges in folding collapse mechanism of crash, which leads to energy absorption of the crash box Furthermore, a modified formulation for the topology optimization was suggested to overcome drawbacks of the ESL method to capture dynamic effects of crash. By applying the obtained ESLs and the modified topology optimization formulation, an efficient topology of a thin-walled box structure that can absorb crash energy was obtained. In axial crushing, major energy absorption is due to generation of continuous folding of the walls, which is the result of plastic buckling. Since the most important area in plastic buckling that carries load and absorbs energy is formed by the plastic hinge lines, the finite elements related to these areas are very critical and need to be strengthened and other areas between two hinge lines can be removed in the optimum topology of the crash box.

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Title: Polyhedral Smoothed Finite Element Method for Thermoelastic and Thermal Contact Analysis

Author(s): *Hobeom Kim, Seyoung Im, *KAIST*.

Thermoelastic and thermal contact analysis by means of three-dimensional polyhedral elements based on smoothed finite elements method (S-FEM) are studied. The S-FEM is classified into several method depending on the way of constructing the smoothing domain: such as nodal cell-based smoothed FEM (CS-FEM ND), node-based smoothed FEM (NS-FEM), and edge-based smoothed FEM (ES-FEM). The S-FEM can realize polyhedral element easily because the shape function is constructed implicitly based on the linear point interpolation and the gradient smoothing technique is applied. Therefore, the stiffness formulation for polyhedral element is more efficient than any other polyhedral FEM. For the thermoelastic analysis, we proposed the method to calculate the fictitious thermal force in polyhedral element due to the thermal strain. The performance of CS-FEM, NS-FEM and ES-FEM using polyhedral elements is compared with one another and the conventional FEM using hexahedral and tetrahedral element. Numerical examples show that the polyhedral smoothed finite element method for thermoelastic analysis is excellent. This method is extended to thermal contact analysis involving nonmatching interface. For this kind of analysis, the method using the polyhedral S-FEM with node-to-node contact scheme is proposed. The polyhedral element with additional nodes and faces is implemented as a transition element for transforming nonmatching interface into matching interface and node-to-node contact scheme is excellent choice for this treatment. The proposed scheme passed the patch test unlike surface-to-surface or node-to-surface contact scheme available from the Abaqus. To verify the proposed scheme, numerical solutions of this method are compared with those from other methods. In addition, the proposed method has turned out to be useful for moving heat source and thermomechanical contact problems.

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Title: Dynamic Finite Element Analysis of Underwater Pipeline under Regular and Irregular Waves

Author(s): *Hyun-Seok Kim, Byoung Wan Kim, Bo-Woo Nam, Kangsu Lee, *KRISO*.

Underwater pipeline has been globally utilized during past decades to carry oil and gas from offshore wellheads to coastal facilities due to its cost-effectiveness on the transportation of hydrocarbon resources. It is known that during the installation process, pipeline suffers high level of stresses. These stresses acting on pipeline may lead to failure of it and further may require entire replacement of the pipeline due to difficulties of underwater repair. Furthermore, underwater pipeline encounters various type of external loadings originated from wave, current, and sea-bed contact, etc. Therefore, a rigorous analysis on pipeline laying procedure which takes account of all the aforementioned conditions is necessary to prevent costly failures. To elucidate the behavior of underwater structures, dynamic nonlinear coupled analysis utilizing catenary element and FEM (Finite Element Method) is performed. In the catenary structure, equilibrium position of itself is determined by subjected tension which is reciprocal with geometry and position. Furthermore, the behavior of catenary is geometrically nonlinear since forces acting on the catenary structure are also dependent on geometry. Due to the consideration of geometric nonlinearity, iteration procedure is required for each time step to obtain the solution which result in high computational cost. In this research, we propose a computationally efficient dynamic analysis method for underwater pipeline during installation by utilizing equilibrium state of catenary at initial configuration and FEM based linear beam element. The proposed method attains efficiency by the linearity of beam element that reduces iterations while acceptable accuracy is retained by imposing catenary structure in finding initial geometry and pretension of pipeline. Effect of sea-bed contact and underwater drag forces is obtained by equivalent spring-damping model and Morison formula. Behavior of underwater pipeline and water particle motion due to wave and current are coupled by considering relative speed between them in Morison formula. Efficiency and accuracy of the proposed method is shown through a comparative study with results from FEM based catenary structure analysis under regular and irregular waves. Applicability of the proposed method for safety design of underwater pipeline is also discussed by analyzing maximum characteristic values and RMS (Root Mean Square) values. B.W. Kim, H.G. Sung, S.Y. Hong, H.J. Jung, Finite element nonlinear analysis for catenary structure considering elastic deformation, Computer Modeling in Engineering & Sciences, 63(1): 29-45, 2010.

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Title: Applying Projection-Based Reduced-Order Modeling to the Constrained System with Lagrange Multipliers

Author(s): *Euiyoung Kim, Maenghyo Cho, *Seoul National University*.

It is common that the analysis of an engineering problem to have constraints on its solution variables. Two methods, the Lagrange multiplier method and the penalty method, are frequently applied to impose the constraints on a number of specified degrees of freedom of the solution fields. In this research, attention is paid to the case of the Lagrange multiplier method. The main topic is the application of the projection-based reduced-order modeling to the system with Lagrange multiplier method. To apply reduced-order modeling while preserving the constraint equations, the proposed approach utilizes Lagrange multiplier method after the systems are reduced. This is the reversed order compared to the conventional approaches where the Lagrange multiplier method is applied first. In the conventional approaches, the reduced coordinate is composed as a unit. It cannot be separated into the constrained and the unconstrained parts. Thus, the constraint equations cannot be added to the reduced model. To tackle this problem, the reduced-order modeling using the local reduced-order bases, which constructs reduction modes separately for the divided domains, is adopted. The displacement solutions are divided into the constrained parts and the non-constrained parts, which are reduced with two different reduction modes; the transformation matrices for the reduction are constructed separately for the degrees of freedom with and without the enforcement of constraints. This makes the constrained part be treated separately from the unconstrained part even in the reduced system so that Lagrange multiplier method can be applied. In the proposed approach, therefore, the Boolean matrix for the Lagrange multiplier method is not reduced, which gives the stability and the accuracy to the solution process. A number of numerical examples that include linear and non-linear structural dynamic analyses with multiple constraints with the Lagrange multiplier method are performed to verify the proposed method. [1] Amsallem, D., Zahr, M. J., & Farhat, C. (2012). Nonlinear model order reduction based on local reduced order bases. International Journal for Numerical Methods in Engineering, 92(10), 891-916. [2] Balajewicz, M., Amsallem, D., & Farhat, C. (2015). Projection■based model reduction for contact problems. International Journal for Numerical Methods in Engineering. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korean government (MSIP) (No. 2012R1A3A2048841)

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Title: Free Energy Calculation and Ghost Force Correction for Hot-QC

Author(s): *Woo Kyun Kim, *University of Cincinnati*; Ellad Tadmor, *University of Minnesota*.

Hot-QC is the finite temperature version of the quasicontinuum (QC) method in which the domain is partition into continuum and atomistic regions. It has been shown that hot-QC reproduces equilibrium properties of fully-atomistic systems including the TST (transition state theory) transition rate so that it can be used to study quasistatic transition events between metastable states. In the original hot-QC method, the free energy in continuum regions is computed using the local harmonic (LH) approximation in which the off-diagonal terms in the Hessian matrix are neglected. To test the accuracy of the LH approximation in hot-QC, we have implemented the quasi-harmonic (QH) method where the full-Hessian matrix is considered. We compare the LH and QH approximation results for various systems including bcc crystals. We also investigate the effect of ghost forces (numerical artifacts appearing at the continuum-atomistic interface) in hot-QC simulations. For static QC, ghost forces can be addressed using a dead-local correction. We test the effectiveness of this approach at finite temperature for both the LH and QH approximations.

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Title: Sensitivity of Mechanical Properties to the Microstructure of Cement Paste Using FOSM Method

Author(s): *Jisu Kim, Tongseok Han, *Yonsei University*.

Concrete properties are generally affected by material characteristics such as porosity and void clustering [1]. Even with the same porosity, the mechanical properties of concrete can be different from each other. The void distribution (micro-structural characteristics) is strongly related to the mechanical properties of porous material. The purpose of this study is to estimate the sensitivity of the mechanical properties of the cement paste to the microstructural characteristics and to develop a methodology for determining the representative volume element (RVE) size of the porous material. The sensitivity analysis is conducted using the first-order second-moment (FOSM) method to estimate the effect of the void distribution of a cement paste specimen on its mechanical properties [2]. Using this method, the sensitivity of the microstructural characteristics on mechanical properties of cement paste can be evaluated. To obtain the microstructural characteristics of cement paste, a virtual specimen is generated from the micro-computerized tomography (micro-CT) images [3]. From the analysis, it is concluded that the sensitivity analysis with multiple characteristics of microstructures can be used to evaluate the effect of the microstructural characteristics on the mechanical properties, and to determine the RVE size of materials. [1] Mindess, S., Young, J. F., Darwin, D. Concrete, 2nd ed., Prentice Hall: U.S.A., 2003, 57-80. [2] Ang, A. H. S., Tang, W. H. Probability Concepts in Engineering: Emphasis on Applications to Civil and Environmental Engineering, 2nd ed., John Wiley and Sons: U.S.A., 2007, 180-189. [3] Chung, S.-Y., Han, T.-S., Kim, S.-Y., Lee, T.-H. Investigation of the permeability of porous concrete reconstructed using probabilistic description methods. Construction and Building Materials 2014, 66, 760-770.

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Title: A Nonlocal Higher-Order Zig-Zag Theory Based on a Strain Gradient Elasticity

Author(s): *Jun-Sik Kim, *Kumoh Nat'l Inst Tech*.

In this paper, a strain gradient elasticity is adopted to consider the thickness length scale effect in laminated composites, which was proposed by Mindlin (1964). As the name suggested, it considers the strain gradients with respect to in-plane and thickness directions. Most research has been focused on the in-plane gradient effects, since the thickness dimensions of plate and shell structures are relatively small. However the laminated composite structures may have a strong heterogeneity through the thickness especially when they are designed to have composite couplings. Such investigations are very rare in the literature. The main objective of this paper is to properly embrace the thickness length scale effect (or thickness heterogeneity) into the higher-order zig-zag theory. The results obtained are assessed in terms of layup sequence, and discussed as compare to a local counterpart.

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Title: Mixed Finite Elements for Nonlinearly Damped Global Tide Models

Author(s): *Robert Kirby, Jameson Graber`, *Baylor University*.

Regional and global tides are modeled by a hyperbolic PDE system, the linearized shallow water equations with Coriolis force and damping due to bottom friction. Many bottom friction models depend nonlinearly on the fluid velocity. However, the nonlinearity greatly complicates the analysis of these problems. We present mixed finite element methods for these equations and describe stability and continuous dependence results that hold for both the semidiscrete and continuous systems. These include effective damping rates for various nonlinearities, rates at which solutions for differing initial conditions approach a global attracting solution, and continuous dependence results on the forcing function. We also discuss a priori error estimates for the finite element solution.

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Title: Cross-Linked Actin Networks: Micro- and Macroscopic Effects

Author(s): *Sandra Klinge, Serhat Aygün, *TU Dortmund University*; Robert P. Gilbert, *University of Delaware*; Gerhard A. Holzapfel, *Graz University of Technology*.

Actin plays a crucial role for the mechanical properties of cell. Together with other proteins, it also drives protrusion, motility and cell division. It is a semi-flexible polymer, i.e. the chains are flexible enough to exhibit considerable thermal bending. The current presentation considers two important aspects of the mechanical modeling of this kind of protein: its microscopic and macroscopic behavior. At the microscopic level, we start with the Holzapfel-Ogden model [1] providing a relationship between the stretch of a single polymer chain and applied tension force. This relationship includes the influence of the physical length of a single chain, its end-to-end distance and the stretch modulus. The model is advantageous as it simulates the so-called “exceptional normal stresses”. This effect is typical of biopolymers and contradicts the Poynting effect observed by rubber-like polymers. The multiscale finite element method [2] is applied to simulate the effective behavior of cell cytoplasm. This method has been intensively used because it is suitable for simulating nonlinear heterogeneous materials with the zero-ratio of the characteristic lengths of scales. The presentation includes results of the macroscopic simulations for different cases of the microstructure. In one case, it is assumed that cytoplasm solely consists of a fine actin-network. In a second case, the cytosol is implemented as an additional phase. [1] M.J. Unterberger, K.M. Schmoller, A.R. Bausch and G.A. Holzapfel, A new approach to model cross-linked actin networks: Multi-scale continuum formulation and computational analysis, J. Mech. Behav. Biomed. Mater., 2013; 22:95—114 [2] S. Klinge and K. Hackl, Application of the multiscale FEM to the modeling of nonlinear composites with a random microstructure, Int. J. Multiscale Comp. Eng., 2012; 10:213–227

14th U.S. National Congress on Computational Mechanics
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Title: Scale-Bridging for Multiscale Modeling of Reactive Materials

Author(s): *Jaroslaw Knap, *U.S. Army Research Laboratory,*; Kenneth W. Leiter, Brian C. Barnes, Richard Becker, Joshua C. Crone, *U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005 USA*.

Over the last few decades, multiscale modeling has become a dominant paradigm in materials modeling and simulation. The practical impact of multiscale modeling depends, to a great extent, on its ability to utilize modern computing platforms. However, since there are no general numerical and computational frameworks for multiscale modeling, the vast majority of multiscale material models or simulations are developed on a case-by-case basis. We seek to formulate an adaptive computational framework for multiscale modeling. Our primary goal is development of scalable numerical algorithms for scale-bridging, the center-piece of any multiscale model. More specifically, we focus on computational methodologies for both spatial and temporal scale-bridging in the context of a two-scale model. We also address the need to significantly reduce the computational cost of multiscale models. We achieve this task via adaptive surrogate modeling. Subsequently, our computational methodologies are evaluated in a two-scale model of an energetic material.

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Title: Microstructure Evolution in Ferroelectrics by Improved Spectral Methods for Computational Homogenization

Author(s): *Dennis Kochmann, *ETH Zurich, Caltech*; A. Vidyasagar, Wei Lin Tan, *Caltech*.

We use an improved Fourier spectral method based on a finite-difference correction for the computational homogenization of polycrystalline ferroelectric ceramics. The improved scheme reduces ringing artifacts and instabilities and is therefore suitable for the simulation of high-contrast scenarios such as composites and polycrystals. Here, we apply the technique to predict the electro-mechanically-coupled behavior of ferroelectrics subjected to combined mechanical and electrical loading. The matrix-free, iterative spectral solution scheme allows for the simulation of large representative volume elements containing thousands of grains which, in turn, contain multiple ferroelectric domains. We compare the predicted material response to in-house experiments performed on lead zirconate titanate (PZT) and discuss the influence of texture and boundary conditions on the material performance.

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Title: A Conforming Kernel for an Agile Design-to-Simulation Process

Author(s): *Jacob Koester, *Sandia National Laboratories*; J.S. Chen, *University of California, San Diego*.

Efficient simulation model development for complex multi-body systems remains a challenge. Meshfree methods, such as the Reproducing Kernel Particle Method (RKPM) [1], have an advantage over the traditional finite element method in that shape functions do not strictly conform to a subdivision of the domain (element). This eliminates the challenge of generating a high quality mesh on complicated geometries, a process that can take months to years [2]. However, the flexibility in construction of shape functions does present new challenges. Domain integration needs re-formulation for balanced accuracy and efficiency [3]. Concave geometries require special consideration so concavities are preserved and unintended discontinuities are not introduced into the approximation space. Part interfaces can be better approximated when the smoothness of the shape functions are properly selected. Computational efficiency and method robustness are affected by the choice of support sizes. In this work, efficiently produced triangulations are used to provide structures to help address the challenges. Reproducing kernel shape function extent is controlled by conforming the kernel function to triangulations. The conforming kernels are generated using C^1 Bernstein-Bezier triangles. The resulting shape functions are C^1 and naturally conform to interfaces and boundaries. Examples utilizing the conforming kernels are shown. [1] W.K. Liu, S. Jun and Y.F. Zhang, Reproducing kernel particle methods, International Journal for Numerical Methods in Fluids, 20, 1081-1106, 1995. [2] M. Hardwick, R. Clay, P. Boggs, E. Walsh, A. Larzelere and A. Altshuler, DART system analysis, SAND2005-4647, Sandia National Laboratories, Albuquerque, NM, 2005. [3] J.S Chen, M. Hillman and M. Rüter, An arbitrary order variationally consistent integration for Galerkin meshfree methods, International Journal for Numerical Methods in Fluids, 95, 387-418, 2013. *Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Projection-Based Topology Optimization: Recent Advancements and Connections to Manufacturing

Author(s): Mikhail Osanov, James Guest, *Saranthip Koh, Josephine Carstensen, *Johns Hopkins University*.

Projection-based topology optimization algorithms have proven effective in achieving clear (0-1) material distributions in density-based topology optimization, while simultaneously enabling the application geometry-based manufacturing constraints. In this talk we will review the fundamental link between projection-based methods and manufacturing, and present new capabilities using the projection-based framework. These include extensions of existing methods to three dimensions, including projection-based algorithms for length scale control in 3D and embedded fibers in 3D printed polymers. Typical benchmark problems are solved in two and three dimensions, and optimized topologies can be transferred to fabrication to illustrate the strong connection between projection and manufacturing.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Solidification Analysis of Ni Based Superalloy Melted by Electron Beam for Additive Manufacturing

Author(s): *Yuichiro Koizumi, Yushi Ohno, Zhao Yufan, Akihiko Chiba, *Tohoku University*.

Electron beam melting (EBM) has attracted attention not only as net-shaping process but also as a revolutionary materials processing technique. In EB powder bed fusion process in which metal powder is melt and solidified selectively by scanning electron beam. EBM process under suitable conditions can form nearly completely dense bodies in contrast to the conventional powder sintering. Controlling microstructures by EBM has been studied intensively in recent years. It has been proposed that microstructure can be predicted by a solidification map because solidification microstructure is determined by temperature gradient (G) and solidification rate (R). However, G and R cannot be measured and controlled directly during EBM process. In order to predict microstructure on the basis of solidification map without manufacturing objects, we need to identify the relationship between process parameters (power: P, scan speed: V) and solidification parameters (G, R) by simulation. The purpose of this study is to construct the new guideline for controlling microstructure by EBM using a Ni-based super alloy as a typical material for which the control of microstructure depending on parts is anticipated to contribute to the improve the performance of gas turbine blade. We used an Arcam A2X EBM system to conduct single bead (without powder) and single bead multi-layer experiments (with powder) on Ni based superalloy Rene80 plate under various conditions (P and V). In the single bead experiments, two types of experiment with or without preheating (950 °C) were conducted to investigate the influence of preheating. G and R at the solid/liquid interface were calculated by computational thermal-fluid dynamics (CtFD) simulation and solidification map was constructed. The model for simulating the melting and solidifying behavior of powder bed was made by a discrete element method (DEM) simulation of the powder raking process. In the single bead experiments, epitaxially and non-epitaxially grown columnar grain perpendicular to the fusion line and nucleation of fine grain along the fusion line of bead were observed. Epitaxial growth and nucleation of fine grain were prominent without and with preheating, respectively, indicating that solidification microstructure depends on the preheating greatly. The simulation revealed that the change of solidification microstructure is due to low G/R resulting from the decrease in temperature gradient by preheating. Solidification map of Rene80 was obtained by the novel method in which the set of G and R on each position of melt pool calculated by CtFD simulation was associated with microstructure determined by EBSD.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: An Explicit Scheme with Local Time Stepping for One-Dimensional Discontinuous Wave Propagation in Heterogeneous Solids

Author(s): *Radek Kolman, *Institute of Thermomechanics*; Sang Soon Cho, *Korea Atomic Energy Research Institute*; Jose G. Gonzalez, *Universidad de Sevilla*; K.C. Park, *University of Colorado at Boulder*; Arkadi Berezovski, *Tallinn University of Technology*.

In this contribution, we focus on accurate finite element modelling of discontinuous wave propagation in an elastic heterogeneous bar. As it is known, the standard explicit time scheme in finite element analysis is not able to ensure accuracy of stress distribution through meshes with different local Courant numbers for each finite element. Moreover, the finite element method produces dispersion behavior and spurious oscillations of stress components. For that reason, a two-time step explicit scheme based on modification of the central difference method with local time stepping and pullback interpolation is suggested for elimination of spurious oscillations and reflections [1]. The nominated scheme is tested on benchmarks for discontinuous wave propagation in layered and functionally graded bars. At the end, numerical results are compared with suitable analytical data and results obtained by the finite volume method. [1] Park, K.C., Lim, S.J. and Huh, H. (2012) A method for computation of discontinuous wave propagation in heterogeneous solids: basic algorithm description and application to one-dimensional problems. International Journal of Numerical Methods and Engineering, 91, 6, pp. 622-643. Acknowledgement The work R. R. and A. B. was supported by the Centre of Excellence for Nonlinear Dynamic Behaviour of Advanced Materials in Engineering CZ.02.1.01/0.0/0.0/15_003/0000493 (Excellent Research Teams) in the framework of Operational Programme Research, Development and Education, and also by the bilateral project No. ETA-15-03. The work of R. R. was supported by the grant project Nos. 16-03823S and 17-22615S of the Czech Science Foundation within institutional support RVO:61388998.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Accurate Wall-Adapting Local Eddy Viscosity Simulation of a Low-Reynolds Straight-Blade Vertical Axis Wind Turbine

Author(s): *Matin Komeili, Marius Paraschivoiu, *Concordia University* .

Application of advanced large eddy simulation (LES) methods, especially in the near wall regions, along with the recent progress in high performance computing have enabled scientists and engineers to accurately simulate low to moderate Reynolds number flows. The interest in these flows have grown considerably in the recent years due to high demands for UAVs and small wind or tidal turbines. The present study is based on using the accurate method of wall-adapting local eddy viscosity (WALE) to simulate complex flows around a single-blade vertical axis wind turbine (VAWT) at a low Reynolds number representative of operating condition on Mars' atmosphere. This finite volume-finite Element code uses second order accurate methods both in time and space in order to discretize the compressible Navier-Stokes equations. A wiggle detector method also is employed to minimize the artificial numerical dissipation. In addition, Arbitrary Lagrangian Eulerian (ALE) technique is used to account for the grid motion. Two blade's profiles are chosen, one is an almost symmetric blade close to the NACA0012 and the second is chambered profile. The local Reynolds number varies between 18000 to 30000, and Mach number, based on free stream velocity, is 0.35. The VAWT is tested at a fixed tip speed ratio (TSR=0.38). The grid is extended by 10% of chord to build a three dimensional domain. The first grid point away from the blade's surface is considered such as Y+< 1 for the entire blade path. The dynamic stall sensitivity of the flow is shown by comparing the results for the two profiles. We specifically focus on finding the azimuthal location when the dynamic stall vortex separates from the leading edge and convects downwards on the airfoil. This location depends on the Reynolds number, the relation between the angle of attack and the airfoil geometry. In this paper, this location is analysed with the use of the highly resolved LES code proposed. This important fundamental work can allow the turbine to operate at high torque conditions and therefore be more efficient.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Microseismic Wave Simulation Using GFEM Enriched Phantom Node Method

Author(s): *Mohammad Komijani, Robert Gracie, *University of Waterloo*.

Numerical simulation of wave propagation has wide range of applications from Crash Analysis to Hydraulic Fracturing. In Hydraulic Fracturing, seismic emissions occur due to induced fracture propagation and reactivation of natural faults. The Finite element method is known as an effective tool for investigation of boundary value problems. However, spurious wave appear in the solutions to transient wave propagation problems. In high-frequency transient wave simulations spurious oscillations appear in solutions due to polynomial interpolations. These oscillations can result in significant errors in wave pattern. To rectify this issue, a new enriched finite element method has been developed in [1] by incorporating trigonometric interpolation functions. Inspired by the enriched/generalized finite element method introduced in [1], Komijani and Gracie [2] recently developed a new enriched finite element model for wave propagation analysis in cracked media based on a combination of the Phantom Node Method (to model arbitrary fractures and discontinuities) and the Generalized Finite Element Method introduced in [1]. In the present research the PNM-GFEM model developed in [2] has been extended to the porous media. Also, the effect of frictional contact has been modeled based on an Uzawa-type augmented Lagrangian contact approach. Transient hydraulically induced seismic emissions are simulated through a fully dynamic coupled model. Effects of different contact simulation approaches as well as coupled poroelastic solution methods on the stability and convergence of the results will be discussed. References: [1] Seounghyun Ham, Klaus-Jürgen Bathe, A finite element method enriched for wave propagation problems, Computers and Structures 94–95 (2012) 1–12. [2] M. Komijani, R. Gracie, An enriched finite element model for wave propagation in fractured media, Finite Elements in Analysis and Design 125 (2017) 14-23.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Fundamental Basis for Computational Modeling of Contact in Wire Ropes and Knots

Author(s): *Alexander Konyukhov, *Karlsruhe Inst. of Technology*.

Beam-to-beam contact can be dually described depending on the scale as curve-to-curve contact or as surface to surface contact. The surface-to-surface (STS) contact algorithm describes the interaction between beams as interaction between two surfaces and in the nominal case requires a continuum description of the beams in terms of solid finite elements, which is computationally expensive. The curve-to-curve (CTC) contact algorithm is rising/generated from the curve to curve closest point projection (CPP) procedure determining a minimal distance between curves. The existence and uniqueness criterion of the CPP procedure has been formulated already in earlier publications. Thus the current contribution is focusing on the detailed analysis of this criterion, namely the case of multiple solutions of the CPP in the case of ``parallel curves``. It is shown that the CTC contact algorithm cannot be applied for general parallel curves, which can be generated in an arbitrary range of angles between the tangent lines -- this case including any wire ropes and also knots connection. For this case a new so-called Curve-To-Solid Beam (CTSB) contact algorithm is developed. This algorithm requires a special Solid Beam finite element and, therefore, is combining the advantages of existence and uniqueness of the CPP for surfaces contact together with the flexibility of application to beam-to-beam contact. The possible applications of various contact pairs -- Surface To Surface, Curve To Curve and Point To Curve are revised in the contribution based on the existence and uniqueness of the corresponding CPP procedures. A special case with "parallel tangent`` vectors is investigated numerically and is considered from the perspective of the classical Hertzian contact for cylindrical bodies. It is found numerically that the corresponding length of a contact zone is well correlated with the Hertz theory. A possible application for wire ropes of the developed strategy -- Solid Beam finite element plus Curve To Solid Beam contact algorithm -- is analyzed numerically.

14th U.S. National Congress on Computational Mechanics
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Title: FSI Framework for Wind Energy and Aerospace Engineering Applications: from Unsteady Aerodynamics to Damage Prediction

Author(s): *Artem Korobenko, *University of Calgary*.

A Fluid-Structure Interaction (FSI) framework for aerospace composite structures is presented. The framework is composed of Variational Multiscale (VMS) methods for aerodynamics posed on a moving domain and thin-shell structural mechanics formulation augmented with progressive damage model for multilayer composites. The key constituents of the framework are presented, including the coupling strategies, in a context of computational analysis of multiple wind turbines in atmospheric boundary layer flow and unmanned-air vehicles under different maneuvers.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Condition Assessment and Prognosis Using Fluid-Structure Interaction Within a Reduced-Order Model Tracking Inversion Framework

Author(s): *Justyna Kosianka, Wensi Wu, Christopher Earls, *Cornell University*.

It is essential to identify damage within a structure as early as possible in order to propose corrective measures to prevent mechanical failure – ultimately extending service life. Such damage detection can be effected through non-destructive means that employ the updating of a physics model describing the system of interest. The resulting inverse problem is concerned with locating and characterizing the damage, by considering the structural dynamic response, before and after the onset of damage. Such model-based approaches also afford prognosis potential; as a calibrated physics model is subsequently available for the damaged system. In this work, a partitioned fluid-structure forward modeling capability is developed from combining an open source CFD tool (OpenFOAM) with an open source CSD solver (CU-BEN) in a tightly coupled framework that affords stable solutions. CU-BEN, an in-house transient dynamic finite element software for structural applications, includes both geometric and material nonlinearity within its structural element formulations, in support of Newton-Raphson and modified spherical arc-length nonlinear solution strategies. Additionally, numerical damping (important for stabilizing FSI solutions) is achieved through an implementation of the generalized-alpha method. Within the context of inversion, the FSI forward model is evaluated on a series of plausible (physically inspired) “damaged” states to create an offline library of modeled damaged responses. These responses are expressed in compressed form through proper orthogonal modes and subsequently represented as points on a certain Reimannian manifold. From this off-line library of compressed response representations from the high-fidelity FSI model, a surrogate model is constructed by “interpolation” on the nonlinear Reimannian manifold to “fill in the gaps” for damage contexts not explicitly contained in the library, but required as part of the inversion. This subsequent online inversion is performed through a genetic algorithm to converge upon the most probable damage estimate within our manifold, so as to match our observed data. A test model of a flag secured to a bluff body post subjected to a one-sided jet-like flow will be used as a demonstration of this method. The damage detection inversion will identify a crack location and length at the root of the structure.

14th U.S. National Congress on Computational Mechanics
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Title: Optimal Quotient Iterations for Large Generalized Eigenvalue Problems

Author(s): Marko Huhtanen, *Vesa Kotila, *University of Oulu, Finland*.

The celebrated Rayleigh quotient iteration (RQI) is a standard approach to iterative solution of eigenvalue problems. For Hermitian eigenvalue problems, RQI has been regarded as optimal due to its cubic convergence, but generalizations to non-Hermitian or generalized eigenvalue problems (GEP) have encountered less success. In this presentation, a new iterative method for solving GEP natively is suggested that outperforms RQI with regards to speed. First, a measure of optimality for a choise of vector projection of GEP is introduced, which leads to a new quotient for approximation of the eigenvalue when an approximate eigenvector is given. Combined with a modified inverse iteration to have a an updated eigenvector, an iterative method is devised which is cubically convergent for a class of GEP's, including the standard Hermitian case. Preconditioning techniques are introduced to steer the iteration to a specific part of the spectrum. The setup is such that no transformation to a standard eigenvalue problem takes place, which supports inaccurate solving of eigenvectors. By using optimization techniques in a subspace generated by a sequence of approximate eigenvectors, monotonic convergence can be guaranteed.

14th U.S. National Congress on Computational Mechanics
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Title: A Parallel Fictitious Domain Method for Fluid-Structure Interaction Based on Pseudo - L2 - Projections

Author(s): *Rolf Krause, Maria Nestola, Patrick Zulian, *USI Lugano*.

The use of variational approaches for the stable information transfer between non-matching meshes along surfaces or overlapping meshes in volumes, represents an essential ingredient for the numerical discretization of coupled multi-physics or multi-scale problems. In this talk, we present an approach for fluid-structure interaction which is based on an immersed boundary approach combined with a pseudo-L2 projection. We employ the finite-element method for discretizing both the equations of the solid structure and the fluid flow and base the information exchange between both on variational transfer in the volume. While the fluid flow is computed on a background mesh, the solid is moving "on top" of the fluid mesh. This allows for computing large deformations without the need of remeshing the fluid. The realization of the variational transfer leads to some technical difficulties in the parallel approach, in particular when the associated meshes are distributed arbitrarily onto different processors. There, the situation becomes even more complicated, since the neighboring elements have to be identified in a global parallel search before the quadrature can be carried out. In this talk we describe in details the approach adopted to solve the FSI problem as well as the main ingredients to get a stable transfer operator between non-matching associated meshes.

14th U.S. National Congress on Computational Mechanics
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Title: Stability Conditions for Variational Formulations Based on Multi-Field Saddle Point Problems

Author(s): *Andreas Krischok, Christian Linder, *Stanford University*.

It has been known for decades that mixed problems with a saddle point variational formulation can suffer from instabilities if the chosen approximation spaces do not satisfy the well-known LBB condition [1]. The satisfaction of the condition is mandatory for problems such as Stokes flow, quasi-incompressible elasticity, and poroelasticity due to their similar variational structure and the issue has parallels in topology optimization and electromagnetics. While the identification and satisfaction of critical conditions is quite well understood for these classical two-field problems, novel multi-physics applications with a saddle-point structure in multiple fields deserve a more critical consideration as the identification and satisfaction of stability estimates is far from trivial. We discuss ways to identify critical conditions in systems with a variational saddle point structure in multiple fields and give a special emphasis to mixed methods in gradient-extended plasticity [2] that suffer from instability problems similar to the classical cases mentioned above. Here, in contrast to problems where the classical LBB condition holds, two or more different conditions may have to be satisfied for the corresponding stability estimate to hold. We identify these critical conditions and confirm in numerical tests that existing finite element formulations for mixed gradient-extended plasticity, previously proposed through trial-and-error, are stable. The talk includes an outlook how the development of mixed methods for these kinds of complex systems may be improved by generalizing existing conditions in a broader framework to quickly judge whether a new model is affected by restrictions on the choice of interpolations.
References: [1] D. Boffi, F. Brezzi & M. Fortin. Mixed finite element methods and applications. Springer, Berlin, 2013. [2] C. Miehe, F. Aldakheel & M. Mauthe. Mixed variational principles and robust finite element implementations of gradient plasticity at small strains. Int. J. Numer. Meth. Eng. 94, 2013 1037 –1074.

14th U.S. National Congress on Computational Mechanics
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Title: An Anisotropic Lagrangian Plasticity Model for Semi-Crystalline Polymers at Finite Strains

Author(s): *Martin Kroon, *Linnaeus University*.

The present work concerns modelling of semi-crystalline polymers, such as polyethylene. Semi-crystalline polymers constitute a material group with an increasing industrial importance. Constitutive response (stress-strain relation) as well as fracture properties are of great importance for this class of materials. We propose an anisotropic plasticity model for semi-crystalline polymers, formulated in the reference configuration (Lagrangian formulation). In addition to plasticity, the model accounts for effects of viscoelasticity. The model is evaluated using uniaxial tensile tests, where polyethylene sheets are tested. The model is able to predict the hardening and rate-dependency observed in the experiments very well. Numerical examples are also presented, where the model is applied to a few different geometries.

14th U.S. National Congress on Computational Mechanics
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Title: Towards an Adaptive Discontinuous Galerkin Storm Surge Model

Author(s): *Ethan J. Kubatko, *The Ohio State University*.

In this presentation, we will discuss the initial development and implementation of adaptive mesh refinement (AMR) capabilities into an existing discontinuous Galerkin shallow water equation model (DG-SWEM). DG-SWEM was developed within the ADCIRC (Advanced CIRCulation) modeling framework, which is extensively used for simulating hurricane storm surge - an area of application where AMR would be particularly beneficial, offering an efficient and effective means of resolving, for example, the hydrodynamic effects of rapidly varying wind and pressure fields, the changing state of flood protection systems and evolving inundation patterns. Preliminary numerical results will be presented, and we will discuss some of the challenges involved in moving forward, which include the implementation of efficient data structures for unstructured meshes, the development of interpolation strategies that aim to conserve mass and momentum when coarsening and refining the mesh, and the use of effective dynamic load balancing techniques in parallel computing environments.

14th U.S. National Congress on Computational Mechanics
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Title: A Moving Contact Line Model for Immiscible Multiphase Flow Problems Using the Conformal Decomposition Finite Element Method

Author(s): *Alec Kucala, David Noble, Mario Martinez, *Sandia National Laboratories* .

Two immiscible fluids in chemical equilibrium form a common interface along a solid surface, the location of which is commonly referred to as the contact line. The equilibrium angle at which these three-phases meet is characterized as the static contact (wetting) angle and is a function of surface geometry, intermolecular forces, and interfacial surface energies manifested as interfacial tension. This static configuration may become perturbed due to external force imbalances (mass injection, pressure gradients, buoyancy, etc.) and the contact line location and interface curvature becomes dynamic; commonly classified as a moving contact line (MCL) problem. The macroscale movement of the contact line is dependent on the molecular interactions occurring at three-phase interface, however most MCL problems require resolution at the meso- and macro-scale. Therefore, a phenomenological model must be developed to account for the microscale interactions, as resolving both the macro- and micro-scale would render most problems computationally intractable. Here, a model for the moving contact line is presented as a weak forcing term in the Navier-Stokes equation and applied directly at the location of the three-phase interface point. The moving interface is tracked with the level-set method and discretized using the conformal decomposition finite element method (CDFEM), allowing for the surface tension and the wetting model to be computed at the exact interface location (sharp interface method). A variety of verification test cases for simple two- and three-dimensional geometries is presented to validate the current model. Evidence of grid independence is also presented when a proper scaling for the slip length is chosen. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
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Title: Constitutive Modeling of Human Brain Tissue

Author(s): Silvia Budday, Paul Steinmann, *U of Erlangen Nuremberg*; Gerhard Sommer, Gerhard A. Holzapfel, *TU Graz*; *Ellen Kuhl, *Stanford*.

Constitutive models of ultrasoft materials like the human brain are highly sensitive to regional and temporal variations and to the type of loading. While recent experiments have shaped our understanding of the time-independent, hyperelastic response of human brain tissue [1], its time-dependent behavior under various loading conditions remains insufficiently understood [2]. Here we combine cyclic and relaxation testing under multiple loading conditions, shear, compression, and tension, to understand the rheology of four different regions of the human brain, the cortex, the basal ganglia, the corona radiata, and the corpus callosum [3]. We establish a family of finite viscoelastic Ogden-type models and calibrate their parameters simultaneously for all loading conditions. We show that the model with only one viscoelastic mode and a constant viscosity captures the essential features of brain tissue: tissue nonlinearity, pre-conditioning, hysteresis, and tension-compression asymmetry. With stiffnesses and time constants of $\mu\propto$=0.7kPa, μ1=2.0kPa, and τ1 = 9.7s in the gray matter cortex and $\mu\propto$=0.3kPa, μ1=0.9kPa and τ1 = 14.9s in the white matter corona radiata combined with negative parameters $\alpha\propto$ and α1, this five-parameter model naturally accounts for pre-conditioning and tissue softening. Increasing the number of viscoelastic modes improves the agreement between model and experiment, especially across the entire relaxation regime. Strikingly, two cycles of pre-conditioning decrease the gray matter stiffness by up to a factor three, while the white matter stiffness remains almost identical. These new insights allow us to better understand the rheology of different brain regions under mixed loading conditions. Our family of finite viscoelastic Ogden-type models for human brain tissue is simple to integrate into standard nonlinear finite element algorithms. Our simultaneous parameter identification of multiple loading modes can inform computational simulations under physiological conditions, especially at high strain rates where time-dependent effects are critical. Ultimately, understanding the rheology of the human brain will allow us to better predict neurosurgical outcomes, determine improved injury criteria, and design smart protection systems. References [1] Budday S, Sommer G, Birkl C, Langkammer C, Hayback J, Kohnert J, Bauer M, Paulsen F, Steinmann P, Kuhl E, Holzapfel GA. Mechanical characterization of human brain tissue. Acta Biomaterialia. 2017, 48:319-340. [2] de Rooij R, Kuhl E. Constitutive Modeling of Brain Tissue: Current Perspectives. Applied Mechanics Review. 2016, 68:1-16. [3] Budday S, Sommer G, Steinmann P, Holzapfel GA, Kuhl E. Rheological characterization of human brain tissue. submitted for publication.

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14th U.S. National Congress on Computational Mechanics
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Title: A Floating Node Method for the Crack Growth Analysis of Brittle Materials

Author(s): *Sachin Kumar, *Indian Institute of Technology Ropar, India*; L.H. Poh, *National University of Singapore, Singapore*; B.Y. Chen, *Institute of High Performance Computing, Singapore*.

All structures/components are subjected to some kind of loading. In some cases, these loads might be applied intentionally or sometimes accidently. Thus, it is essential to analyze the fracture behavior of such components to avoid the hazardous situations. In last few decades, several numerical techniques have been proposed i.e. finite element method, meshfree methods, extended finite element method and phantom node method for the fracture analysis of components. While these techniques are able to capture the fracture behavior of structures, there exist several limitations, e.g. requirement of remeshing in finite element method during crack propagation, error in mapping of crack geometry from physical to natural space in phantom node method and the need of enrichment functions in the extended finite element method. This paper presents a new approach suitable for the modeling of discontinuities within a finite element. The floating node method, first developed for modeling the fracture behavior of laminate composites, is here extended for the generic fracture of brittle materials. The architecture of the proposed technique is similar to the phantom node method (which is equivalent to XFEM with Heaviside enrichment only), and the solution of it is equivalent to local remeshing within the cracked element. In this approach, additional nodes are introduced to model the discontinuities. These additional nodes, known as floating nodes, are deactivated until unless a discontinuity develops within a finite element. These floating nodes do not coincide with the real nodes, and their locations within each element is determined from the discontinuity within the said element. The floating node method thus models the discontinuities without modifying the initial mesh and geometry, thus making it computationally more efficient. Additionally, the proposed method is particularly suitable for modelling weak and cohesive interfaces. We consider several benchmark examples of fracture mechanics. The results shows that the floating node method can model the entire failure behavior of a component, from crack initiation to final failure.

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Title: Simultaneous Optimization of Topology and Pointwise Constitutive Properties through Multi-Variable SIMP

Author(s): *Tej Kumar, Krishnan Suresh, *U.Wisconsin, Madison*.

The advent of 3D printing has enabled the possibility of fabricating complex topologies with custom designed microstructures. However, efficient computation of such designs is however an open challenge. Here, we propose a unified strategy for the simultaneous optimization of the topology, and the pointwise constitutive property for microstructural design. The unified strategy involves generalization of the classic Solid Isotropic Material with Penalization (SIMP) method. Specifically, instead of assigning one design variable per element, we assign multiple variables. For example, in 2D, each element is assigned one density variable for topology control, and 4 additional variables for the control of the four (orthotropic) constitutive properties, namely C11, C22, C12 and C33. Similarly, in 3D, we assign one topology-control variable and 9 additional constitutive property variables per element. These additional variables can be constrained to behave in a certain way if desired. The resulting multi-variable SIMP problem can be solved using any optimization method such as MMA. We refer to the resulting map of the material properties as pointwise constitutive property (PCP) map. We show that the PCP map, together with the topology, leads to expected results for classic problems. Since the PCP map yields the required constitutive properties through the domain, it can be used for microstructural design to replicate the desired properties. For example, the microstructures can be designed (in parallel) by minimizing the Frobenius norm of the difference in constitutive properties. Alternately, one could select from a set of predefined microstructures to best match the desired constitutive properties.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Coupled Iso-Geometric Analysis (IGA) and Peridynamics Method for Ship Structural Analysis

Author(s): *Shih-Mo Kuo, Pai-Chen Guan, *National Taiwan Ocean Univ.*.

The thick plates (over 20 mm) are the most important structural member for the construction of ultra large ships and marine structures. One of the most essential design requirement for thick plates is the crack generation and accumulation, which greatly affect the reliability and safety of the structure. Therefore, the design rule usually demand shipyard to provide documents regarding crack accumulation for later inspection. The main purpose of this research is to develop a numerical tool that could model the crack formation and propagation on ship. The method we proposed is the adaptively coupled isogeometric analysis (IGA)-peridynamics method. The IGA method is recently developed method in the field of solid mechanics. It is currently one of the most robust method for solving problems with complex surface geometry and deformation, which is a perfect match for the ship structural analysis. On the other hand, peridynamics is a new particle based method that can solve the crack problem efficiently. To couple these two methods, we introduced three possible approaches: subdomain interface, overlapping interface and smoothed coupling. In subdomain interface method, the IGA domain and peridynamics domain only share the interface line. We use penalty method to enforce the continuity of displacement on the interface. In overlapping interface method, the coupling zone where the IGA mesh and peridynamics particle overlapping with each other is introduced. The penalty method is also applied in the coupling area to maintain the continuity. The size of the overlapping area is proportional to the wave speed, nodal distance and order of IGA shape functions. In the smoothed coupling method, we introduce smoothed kernel function for the peridynamics particles in the coupling zone. Then we use ramping function to gradually couple the displacement filed by the assumed kernel function and IGA approximation. All coupling methods are tested with the plane wave and complex wave propagation problems. The subdomain coupling leads to more severe non-physical wave reflection while both overlapping and ramping methods give more stable solution in the coupling region.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: 3D Fracture Simulation of Reinforced Concrete Using Damage Model Based on Fracture Mechanics for Concrete

Author(s): *Mao Kurumatani, Yuto Soma, *Ibaraki University*.

We present a method for simulating fracture behavior of concrete and reinforced concrete involving crack propagations in 3D, and demonstrate its performance. Fracture behavior of concrete with crack propagation is analyzed using an isotropic damage model based on fracture mechanics for concrete in consideration of a cohesive zone in the fracture process [1], which is a kind of the energy balance approach in terms of fracture energy. The modified von-Mises criterion, which is also defined as an equivalent scalar strain, is introduced into the damage model to evaluate the initiation and propagation of cracks in concrete. The isotropic von-Mises plasticity model is applied to steel bars. Combining these damage and plasticity models with the finite element analysis enables us to simulate the detailed progressive fracture behavior of reinforced concrete involving crack propagation and plastic deformation in 3D. The MPI parallel computing is also applied to the fracture simulation for performing the numerical analysis of RC structure efficiently. We first explain the modeling of material behavior of concrete and steel, and show the formulation of the damage model for concrete and the plasticity model for steel bars. Several numerical examples are then presented to demonstrate the performance of the method for concrete and reinforced concrete. We also compare the numerical results with the own experimental ones for RC beams with different shear reinforcements in order to demonstrate the validity of the method. The efficiency of parallel computing is also examined in the fracture simulation of RC beams. [1] Kurumatani M, Terada K, Kato J, Koya T, Kashiyama K: An isotropic damage model based on fracture mechanics for concrete, Engineering Fracture Mechanics, Vol.155, p.49-66, 2016.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Structural-Based Computational Model of Tendon-to-Bone Insertion

Author(s): *Sergey Kuznetsov, Hsiao-Ying Shadow Huang, *Department of Mechanical and Aerospace Engineering, North Carolina State University*.

Tendon-to-bone insertions are functionally-graded connective tissues whose anisotropic biomechanical functions depend intimately on the regional biochemical composition and structure [1]. The insertion site provides a gradual transition from soft tendon tissue to hard bone tissue, functioning to alleviate stress concentration at the junction of these tissues [2]. Specifically, dense and highly aligned collagen fibers are characteristic of the tendon side of the junction, and a high density of the mineral hydroxyapatite with randomly distributed collagen fibers is characteristic at the bone side. Inhomogeneity and discontinuities in tissue-level properties at the insertion site manifest in the unique, stress concentration-reducing material behavior at the macro-scale. To better understand how tendon-to-bone insertion performs its function, we developed a computational model of tendon-to-bone insertion implemented in commercial finite element software ABAQUS. We adopted linear elastic and nonlinear anisotropic Gasser-Ogden-Holzapfel model [3] to incorporate collagen fiber dispersion and mineralization concentration. We started with a simplified geometry of tendon-to-bone insertion [2]. A python script was developed to alter the tapered tendon-bone transition zone and to provide spatial grading of material properties, which may be rather complex as experiments suggest. A simple linear interpolation between tendon and bone material properties was first used to describe the graded property within the insertion region. Stress distributions are obtained and compared for spatially graded and various piece-wise materials properties. It was observed that spatial grading results in more smooth stress distributions and significantly reduces maximum stresses. The geometry of the tissue model could be optimized by minimizing the peak stress to mimic in-vivo tissue remodeling. The in-silico elastic models constructed in this work are verified and modified by comparing to our in-situ biaxial mechanical testing results, thereby serving as translational tools for accurately predicting the material behavior of the tendon-to-bone insertions. This model will be useful for understanding how tendon-to-bone insertion functions and may be also useful to planning surgical interventions and developing orthopedic implants. References: [1] G. M. Genin et al, Functional Grading of Mineral and Collagen in the Attachment of Tendon to Bone(2009), Biophysical Journal, Vol.97, 976-986. [2] Y. Liu et al, Mechanisms of Bimaterial Attachment at the Interface of Tendon to Bone(2011), J. Eng. Mater. Technol., Vol.133. [3] T. C. Gasser et al, Hyperelastic Modeling of Arterial Layers with Distributed Collagen Fibre Orientations(2006), J. R. Soc. Interface, Vol.3, 15-35.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Cement Sheath Failure and Interface Debonding Driven by Temperature and Pore Pressure Effects in a Cased and Cemented Wellbore

Author(s): Sergey Golovin, *Lavrentyev Institute of Hydrod*; *Dmitry Kuznetsov, Nicolas Flamant, *Technology Company Schlumberger*; Alexander Valov, *Novosibirsk State University*; Tatiana Rotanova, *Lavrentyev Institute of Hydrodynamics*.

The integrity of cemented annuli of a cased wellbore is an important factor for prevention of fluid migration between permeable layers. The wellbore consists of sections of decreasing diameter. Over each section, the wellbore is cased and cemented such that each cross section consists of three layers: steel casing, cement sheath, and rock. Over the joints where the wellbore's diameter changes, there are two nested casings. The casing is subjected to loads due to the in situ stress in the formation, to the prestress caused by the shrinkage or extension of the cement during settling, and to the stresses during well operations. The combination of these stresses can provoke cracks within the cement or a debonding over the materials' interface. We present results of a mathematical modelling of stresses near the cased and cemented wellbore under the described types of loadings. We use a fully coupled thermo-poro-elastic model that involves the pre-existing stress, the nonuniformity of the in situ stress and the eccentricity of the casing. The plain strain approximation is adopted. The potential failure of the cement sheath is described by the comparison of failure criteria with the critical value. By this, we can find the time instant of the failure and the position of the initial crack. The debonding over the steel/cement or cement/rock interface is described using the continual failure model. We discuss possible scenarios of well exploitation that can cause either the failure of the cement sheath or the debonding and growth of the microannulus over the boundaries. In particular, it is shown that the residue of initial pre-stress due to the cement settling can generate stress of the same order as the in situ geological stress. Pressure of the pore fluid does not play a significant role in the stress distribution for a single-cased well if the steel casing is not perforated. However, for the double-cased wellbore, variations of the pore fluid temperature can result in the high pore pressure of the same order as the stress applied to the inner casing of the wellbore. For noncentered casing or in the case of a high ratio between the maximal and minimal geological in situ stresses, the stress is distributed nonuniformly near the wellbore. We discuss possible locations and mechanisms of the cement failure and fracture propagation.

14th U.S. National Congress on Computational Mechanics
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Title: Error Estimates for Adaptive Isogeometric Analysis of Stokes Problem

Author(s): *Trond Kvamsdal, Abdullah Abdullhaque, *NTNU*; Mukesh Kumar, *College of Charleston*; Arne Morten Kvarving, *SINTEF Digital*.

Error estimates suitable for adaptive isogeometric mixed methods for solving Stokes problem will be presented. We will here compare the use of residual based error estimators with superconvergent patch recovery methods [1]. The adaptive refinement will be based on the use of LR B-splines [2]. The different estimators will be thoroughly tested on problems with (manufactured) analytical solutions. [1] Kumar, M., Kvamsdal, T. and Johannessen, K. A. Superconvergent patch recovery and a posteriori error estimation technique in adaptive isogeometric analysis. Computer Methods in Applied Mechanics and Engineering, 316, pp. 1086-1156, 2017. [2] K. A. Johannessen, T. Kvamsdal, and T. Dokken. Isogeometric analysis using LR B-splines. Computer Methods in Applied Mechanics and Engineering, 269:471–514, 2014.

14th U.S. National Congress on Computational Mechanics
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Title: Modeling of Flow and Scouring under Pipelines by Reproducing Kernel Particle Method

Author(s): *On Lei Annie Kwok, *National Taiwan University*; Pai-Chen Guan, Chien-Ting Sun, *National Taiwan Ocean University*.

Due to the loadings by ocean waves and tidal currents, seabed scour is a serious threat to the offshore pipelines. Scouring is a complex phenomenon as it involves fluid-structure-soil interaction and transport of soil sediments. In this research, a numerical modeling framework based on the reproducing kernel particle method (RKPM) is developed to model the scouring behavior around the pipelines. The ocean wave and tidal flow is modeled by the semi-Lagrangian RK incompressible fluid method (SLRKIF). Under this framework, the conservation of momentum, continuity and energy conservation are solved by the Galerkin weak form of semi-Lagrangian RK shape functions. The pipeline is modeled by the RKPM Mindlin plate formulation. The seabed sediment is modeled by the semi-Lagrangian RK soil code. The interaction of fluid (waves), structure (pipelines) and solid (soil sediment) will be modeled by a new contact algorithm. In this study, effect of wave characteristics, pipeline geometry and spacing, and soil properties on scouring will be evaluated.

14th U.S. National Congress on Computational Mechanics
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Title: Spectral Inverse Iteration for Eigenvalue Problems with Random Coefficients

Author(s): *Mikael Laaksonen, Harri Hakula, *Aalto University*.

In this talk we present an algorithm of spectral inverse iteration for solving eigenvalue problems of elliptic operators with random coefficients. The algorithm is based on the stochastic Galerkin approach with respect to a sparse polynomial basis and, as opposed to the popular nonintrusive schemes such as Monte Carlo simulation and stochastic collocation, no numerical quadrature over the parameter spaces is needed. Normalization of the eigenfunction is performed via solving a nonlinear system of equations defining the Galerkin coefficients. It is possible to extend the algorithm to a spectral subspace iteration with which we can deal with the problematic issue of eigenvalue crossings, i.e., eigenvalues of higher multiplicity. The functionality of our algorithm is assessed mainly through numerical examples. We also briefly discuss the ingredients of an efficient implementation. We use solutions computed by a stochastic collocation scheme as a reference, and demonstrate convergence of our algorithm to these reference solutions. In particular, we aim to demonstrate the key advantages of the Galerkin approach as opposed to collocation. References: [1] H. Hakula, V. Kaarnioja, M. Laaksonen, Approximate methods for stochastic eigenvalue problems, Applied Mathematics and Computation 267, 2015, pp. 664–681. [2] H. Meidani, R. Ghanem, Spectral power iterations for the random eigenvalue problem, AIAA J. 52, 2014, pp. 912–925. [3] R. Andreev, C. Schwab, Sparse tensor approximation of parametric eigenvalue problems, Lecture notes in computational science and engineering Vol. 83, Springer Berlin, 2012, pp. 203–241.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Domain Decomposition for Numerical Integration of Green's Functions for Layered, Transversely Isotropic Soil Media

Author(s): *Josue Labaki, *University of Campinas*.

Models of dynamic soil-foundation interaction such as raft foundations and embedded pile groups often require the derivation of Green's functions corresponding to surface and embedded circular or cylindrical shell loads within transversely isotropic, layered half-spaces. These Green's functions are obtained through the numerical integration of indefinite integrals containing an infinite number of singularities and oscillating-decaying components whose integrals only converge at infinity. There are currently no numerical methods to deal with both characteristics of these integrands. This paper presents a study on the characteristics of integrands of these Green's functions and techniques to decompose the integration domain so that appropriate numerical methods can be applied to each domain. Without loss of generality, the paper considers a Green's function for axisymmetric, time-harmonic cylindrical shell loads within layered half-spaces. The half-space is described by the exact stiffness method [1], in which the stiffness of the layered system is obtained by the linear combination of the stiffness of its constituent layers. This scheme results in displacements of the layered system in the Hankel transformed domain, and must be integrated numerically in order to obtain the corresponding displacements in the physical domain. The integrands in this problem may be divided into two regions, each demanding a specialized integration technique. The first region is characterized by the presence of an infinite number of singularities, which arise from the reflection of elastic waves within the layers in the half-space. This region can be integrated by dividing it at the singularities and integrating within these subregions by adaptive Gaussian quadrature. The second region is characterized by an oscillating-decaying integrand, which can be integrated with Longman's scheme [2]. The value of the Hankel space variable that divides the two regions varies according to parameters of the loading and the constitution of the layered soil. This paper proposes a scheme to find this value through an analysis of the stiffness matrix of the layered soil. The accurate numerical integration of Green's functions is an indispensable component in the formulation of many models of embedded foundations, including the case of elastic piles and pile groups, thick cylindrical foundations, and anchors. [1] Wang YY, Rajapakse RD (1994). An Exact Stiffness Method for Elastodynamics of a Layered Orthotropic Half-Plane. ASME. J. Appl. Mech.; 61(2):339-348. [2] Longman, IM (1956): Note on a method for computing infinite integrals of oscillatory functions. Proc. Cambridge Phil. Soc.; 52: 764-768.

14th U.S. National Congress on Computational Mechanics
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Title: Coupling of Molecular Dynamics and Lattice-Boltzmann on Spatially-Adaptive Grids

Author(s): *Michael Lahnert, Miriam Mehl, *University of Stuttgart*; Takayuki Aoki, *Tokyo Institute of Technology*; Carsten Burstedde, *Rheinische Friedrich-Wilhelms-Universitaet Bonn*.

In modern day simulations researchers have a particular interest in modeling physical, chemical, or biological processes on multiple time and length scales and combine them in a single simulation. One particular example for such an approach are (coarse grained) molecular ensembles embedded in a liquid or gas. This approach may be used to simulate DNA transport through a nano pore or the extraction of dust particles through filter media. To tackle these problems we want to use ESPResSo, which is a very versatile and feature rich molecular dynamics (MD) simulation tool that uses a thermalized D3Q19 implementation of the lattice-Boltzmann method (LBM) on a regular grid to simulate a background flow. This simple spatial discretization prevents the transition to physically more relevant time and length scales. To overcome this problem we want to use adaptive mesh refinement (AMR) to reduce the number of degrees of freedom in the system. As not all regions in the simulation domain have the same relevance to the solution, AMR allows focusing on regions of high interest while reducing computational load in regions where that level of detail is not required. While there are various different approaches to AMR we want to focus on two important aspects: 1) We want to focus on a minimally-invasive integration to preserve as much of the expert knowledge as possible that is already contained in the application. 2) We want the AMR library to be as lightweight and scalable as possible to avoid introducing additional costs. To this end, we choose the forest-of-octrees approach and p4est, an efficient and well scaling grid library. Our contribution consists of three important aspects: First, we extended p4est to be better suited in terms of a minimally-invasive integration into an existing application. Second, we replaced the regular linked-cell and LBM grids in ESPResSo to reduce the number of degrees of freedom in the system. To exploit the embarrassingly parallel nature of the LBM algorithm and because more and more modern super-computers rely on accelerator hardware to achieve their peak performance on the road to Exascale systems, we implemented a GPU implementation of the LBM for our spatially-adaptive p4est-based grid using CUDA. We will show first results of our coupling between LBM and MD as well as upscaling tests of our implementations.

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Title: A Framework for the Modeling of Gypsum Cavity Dissolution Within Geomechanical Studies

Author(s): *Farid Laouafa, *INERIS*; Michel Quintard, *IMFT/INPT/CNRS*.

We are interested in the issue of dissolution of certain soluble rocks, and their geomechanical consequences such subsidence, sinkholes, underground collapse. We will focus on gypsum, although the developed method is usable for salt rocks. In this paper, a large-scale Diffuse Interface Model (DIM) is used to describe the evolution of a gypsum cavity formation induced by dissolution. The method is based upon the assumption of a pseudo-component dissolving with a thermodynamic equilibrium boundary condition. A methodology is proposed based on numerical computations with fixed boundaries in order to choose suitable parameters for the DIM model and hence predict the correct dissolution fluxes and surface recession velocity. Additional simulations were performed to check which type of momentum balance equation should be used. The numerical results did not show a strong impact of this choice for the typical initial boundary value problems under consideration. Calculations with a variable density and Boussinesq approximation were also performed to evaluate the potential for natural convection. The results showed that the impact of density driven flows were negligible in the cases under investigation. The potential of the methodology is illustrated on two large-scale configurations: one corresponding to a gypsum lens contained within a porous rock layer and the other to an isolated pillar in a flooded gypsum quarry. Geomechanical consequences of the dissolution in terms of mechanical stability is evaluated with the help of a simplified geomechanical model. A final case is also studied in which gypsum is replaced by salt to show the applicability of the proposed methodology to a rapidly dissolving material or high solubility. References : H. Luo, M. Quintard, G. Debenest, and F. Laouafa (2012). Properties of a diffuse interface model based on a porous medium theory for solid–liquid dissolution problems. Computational Geosciences, 16:913–932, 2012. H. Luo, F. Laouafa, G. Debenest and M. Quintard (2015). Large scale cavity dissolution: From the physical problem to its numerical solution. European Journal of Mechanics B/Fluids 52, 131–146 J. Guo, F. Laouafa, M. Quintard, (2016) A theoretical and numerical framework for modeling gypsum cavity dissolution International Journal for Numerical and Analytical Methods in Geomechanics vol. 40 (12) p. 1662-1689

14th U.S. National Congress on Computational Mechanics
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Title: Fully Three Dimensional Model of Hydraulic Fracture Propagation

Author(s): Sergey Cherny, *Vasily Lapin, Denis Esipov, Dmitriy Kuranakov, *Inst. Computat. Technol. SBRAS*.

This study is devoted to development and application of the new numerical model of hydraulic fracture propagation proposed in [1]. The model consists of three fully coupled sub-models for three main processes: 1) rock deformation caused by fluid pressure on the fracture surfaces, 2) rock breaking and fracture propagation and 3) fluid flow inside the fracture. Rock deformation in the vicinity of the fracture and the cavity (wellbore with perforations, notches etc.) is described in scope of linear elasticity equations for homogeneous uniform material. Conventional and dual boundary element methods are applied to solve the equations in the model. In [2] a modification of dual boundary element method is proposed. A system of displacement and traction boundary integral equations is written for displacement discontinuity at the points of one side of the fracture and for displacement at the points on the cavity surface. This modification significantly reduces the amount of computation, since approximation of one side of the fracture is required. New implicit formulation of three-dimensional criteria of direction of fracture propagation is proposed. Criteria are written in form of conditions for of stress intensity factor modes I and II that are treated as functions of both kinking and twisting angles. The conditions are combined into one functional that is numerically minimized to obtain the values of the kinking and twisting angles at each point of the fracture front. The Herschel-Bulkley model is used to describe the flow of non-Newtonian fluid and the Reynolds equation is modified for low-compressible fluid flow simulation like it described in [3]. The influence of the fluid rheology and compressibility on the fluid pressure and the fracture form is shown for the case of inclined hydraulically driven penny shaped fracture in the rock under multiaxial load. 1. Cherny S.G., Lapin V.N., Esipov D.V., Kuranakov D.S., Avdyushenko A.Y., Lyutov A.E., Karnakov P.V. Simulating fully 3D non-planar evolution of hydraulic fractures // International Journal of Fracture. - 2016. - P.1-31. 2. Kuranakov D.S., Esipov D.V., Lapin V.N., Cherny S.G. Modification of the boundary element method for computation of three-dimensional fields of strain-stress state of cavities with cracks // Engineering Fracture Mechanics. - 2016. - Vol.153. - P.302-318. 3. Cherny S.G., Lapin V.N. 3D model of hydraulic fracture with Herschel-Bulkley compressible fluid pumping // Procedia Structural Integrity V. 2. – 2016. - P.2479-2486.

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Title: Reduced Order Finite Element Formulation for Vibroacoustic Analysis of Double-Wall Sandwich Panels with Viscoelastic and Piezoelectric Damping Treatments

Author(s): *Walid Larbi, Jean-François Deü, Roger Ohayon, *CNAM Paris France*.

This work concerns the control of sound transmission through double laminated panels using passive piezoelectric shunt technique. More specifically, the system consists of two sandwich panels (each one composed of two elastic faces and a viscoelastic core) with an air gap in between. Furthermore, piezoelectric patches (connected to a resonant shunt circuit) are surface-mounted on the external faces of the structure in order to damp some specific resonance frequencies of the coupled system. Firstly, a finite element formulation of the fully coupled visco-electro-mechanical-acoustic system is presented. This formulation takes into account the frequency dependence of the viscoelastic material, the electro-mechanical coupling of the piezoelectric elements and the elastoacoustic interaction. A modal reduction approach is then proposed to solve the problem at a lower cost. To this end, the coupled system is solved by projecting the mechanical displacement and the pressure unknown on a truncated basis composed respectively of the first real short-circuit structural modes and the first acoustic modes with rigid boundaries conditions. A static correction is also introduced in order to take into account the effect of higher modes. Moreover, due to the fact that only two electrical variables per piezoelectric patch are used (the electric charge contained in the electrodes and the voltage between the electrodes), they are kept in the reduced system. Finally, numerical examples are analyzed to show the efficiency of the proposed reduced order model. References W. Larbi, J.-F. Deü, R. Ohayon, Finite element reduced order model for noise and vibration reduction of double sandwich panels using shunted piezoelectric patches, Applied Acoustics, 108, 40-49, 2016. J.-F. Deü, W. Larbi, R. Ohayon, R. Sampaio, Piezoelectric shunt vibration damping of structural-acoustic systems: Finite element formulation and reduced-order model, Journal of Vibration and Acoustics, 136 (3), 031007, 2014. J.-F. Deü, W. Larbi, R. Ohayon, Piezoelectric structural acoustic problems: Symmetric variational formulations and finite element results, Computer Methods in Applied Mechanics and Engineering, 197 (19-20), 1715-1724, 2008.

14th U.S. National Congress on Computational Mechanics
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Title: Geometric Meshing of Discrete Surfaces

Author(s): *Patrick Laug, *Inria Saclay IdF, France*; Houman Borouchaki, *University of Technology of Troyes, France*.

Most computer-aided design (CAD) systems include a boundary representation (B-rep) where a surface is modeled by a collection of patches, each patch being defined by a function sigma from a parametric domain in R2 to a face in R3. To generate a mesh of such a surface, an indirect approach can be used [1]. In this case, the size and shape of the elements to be generated on the surface are specified by metrics M3, which are converted into metrics M2 in the parametric domain using the first partial derivatives of sigma in order to control meshing in two dimensions. The initial metrics M3 on the surface are either isotropic or anisotropic, and can depend from geometric features to generate a "geometric mesh". To obtain an isotropic geometric mesh, the prescribed size is proportional to the minimum radius of curvature at any point of the surface. For an anisotropic geometric mesh, the prescribed size depends on the two principal curvatures and the two corresponding principal directions. All these geometric features are based on the first and second partial derivatives of sigma. To summarize, the indirect approach for surface meshing needs the evaluation of sigma, its first partial derivatives and possibly its second partial derivatives. In practice, these computations are realized by CAD queries, which in some cases may be time-consuming, non-parallelizable, or return degenerate values. To overcome these problems, a discrete model made up of triangles can be built from the continuous CAD model. Then, an approximation of sigma and it first partial derivatives can be computed efficiently; since the first derivatives are constant on each triangle, they can even be stored to increase speed. The second partial derivatives are null but curvatures can be approximated at each vertex and then interpolated in order to generate an isotropic geometric mesh [2]. We now propose a new approach where the first and second derivatives of sigma are computed at the vertices of the discrete model, based on Taylor expansions. This approach improves efficiency to generate isotropic geometric meshes, and makes it possible to generate anisotropic geometric meshes. [1] H. Borouchaki, P. Laug, P.L. George, Parametric Surface Meshing using a Combined Advancing-Front / Generalized-Delaunay Approach, Int. J. Numer. Meth. Eng. (49)1-2:233-259, 2000. [2] P. Laug, H. Borouchaki, Discrete CAD Model for Visualization and Meshing, 25th International Meshing Roundtable, Procedia Engineering (163)149–161, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: Frictional Contact on a Rigid Obstacle for the Particle-Difference Method

Author(s): Tae-Yeon Kim, *Tod Laursen, *Khalifa University*; Dhafer khalefa Jadaan, Jeong-hoon Song, *University of Colorado at Boulder*.

We present contact algorithms for the particle-difference method (PDM) which is a meshfree point collocation method. The PDM directly discretizes governing equations using the pre-computed approximations. The method incorporates a Taylor expansion with a moving least square approximation to define its shape functions. In contrast to other meshfree methods, the PDM does not require the regularity of the weight function, ensuring the regularity of the shape functions. The method relies on neighboring nodes within a dilation parameter suitable for local refinement and dynamic adaptivity. As a result, the grid can be easily adapted to resolve contact surfaces of the solutions. This study is to apply these advantages of the PDM to frictional contact problems. We present a means of defining frictional contact constraints directly on governing equations for the body contact with a rigid, immobile obstacle. Numerical studies for several benchmark problems in frictional contact are performed to demonstrate the accuracy and efficacy of the method.

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Title: Attenuation of Acoustic Waves and Mechanical Vibrations at Low Frequencies by a Nonlinear Dynamical Absorber

Author(s): *Deborah Lavazec, *Université Paris-Est*; Gwendal Cumunel, Denis Duhamel, *Navier (Université Paris-Est)*; Christian Soize, *MSME (Université Paris-Est)*.

At the present time, the attenuation of acoustic waves and mechanical vibrations at high and middle frequencies is well known and easily done, especially with dissipative materials. However, this attenuation is much more difficult to realize at low frequencies because of the large wavelengths. In the work presented here, we propose to reduce the noise and the vibrations at low frequencies over a broad frequency band by means of nonlinear absorbers allowing a transfer and a dissipation of the energy. These absorbers are randomly arranged in a matrix and have a nonlinear dynamical behavior. The absorber consists of a cantilever beam supporting a concentrated mass at its end. It is designed in order to obtain a nonlinear dynamical behavior in the low-frequency band due to the finite displacements of the beam. This mechanical system is modeled by a mass-spring-damper system with a nonlinear stiffness and a nonlinear damping. Indeed, nonlinearity allows attenuation over a broader frequency band, unlike linear systems which only generate a reduction over a narrow frequency band around the resonance, which makes it possible to reduce the number of absorbers needed for a given attenuation . We will first present the design of the nonlinear absorber optimized using stochastic modeling in order to obtain the most adequate nonlinear response possible. Then, experimental results will be presented as well as their comparisons with the numerical predictions. Then, we present the modeling and numerical homogenization of a beam containing several randomly distributed nonlinear absorbers and their effective dissipation. This will be compared with the results of the experimental analysis of this system.

14th U.S. National Congress on Computational Mechanics
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Title: Multilevel Monte Carlo Methods for Bayesian Inference

Author(s): *Kody Law, *Oak Ridge National Laboratory*.

Bayesian inference provides a principled and well-defined approach to the integration of data into an a priori known distribution, for a posterior uncertainty quantification. The posterior distribution, however, is known only point-wise (possibly with an intractable likelihood) and up to a normalizing constant. Monte Carlo methods have been designed to sample such distributions, such as Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC) samplers. Recently, the multilevel Monte Carlo (MLMC) framework has been extended to some of these cases, so that approximation error can be optimally balanced with statistical sampling error, and ultimately the Bayesian inverse problem can be solved for the same asymptotic cost as solving the deterministic forward problem. This talk will concern the recent development of multilevel SMC (MLSMC) samplers and the resulting estimators for standard quantities of interest as well as normalizing constants, as well as ML particle filters and ensemble Kalman filters.

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Title: Multilevel Monte Carlo Methods for Bayesian Inference

Author(s): *Kody Law, *Oak Ridge National Laboratory*.

Bayesian inference provides a principled and well-defined approach to the integration of data into an a priori known distribution, for a posterior uncertainty quantification. The posterior distribution, however, is known only point-wise (possibly with an intractable likelihood) and up to a normalizing constant. Monte Carlo methods have been designed to sample such distributions, such as Markov chain Monte Carlo (MCMC) and sequential Monte Carlo (SMC) samplers. Recently, the multilevel Monte Carlo (MLMC) framework has been extended to some of these cases, so that approximation error can be optimally balanced with statistical sampling error, and ultimately the Bayesian inverse problem can be solved for the same asymptotic cost as solving the deterministic forward problem. This talk will concern the recent development of multilevel SMC (MLSMC) samplers and the resulting estimators for standard quantities of interest as well as normalizing constants, as well as ML particle filters and ensemble Kalman filters.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Numerical Modeling of High-Temperature Superconductors Using the Discontinuous Galerkin Method

Author(s): *Yann-Meing Law-Kam Cio, Steven Dufour, *École Polytechnique Montréal*.

The improvement of the processes used for the manufacturing of high-temperature superconductor (HTS) based devices allows the design of more compact high-current cables and fault current limiters [1]. Numerical modeling can give an estimate of the alternate current losses which are used for design optimization. The numerical modeling of HTS is challenging. The resistivity of HTS materials is nonlinear and power-law models or the Bean's model must be used. Moreover, a typical HTS wire is composed of a combination of an HTS material and of a normal conducting material, surrounded by air. Each material is characterized by different resistivity models. Most formulations use the magneto-quasistatic condition which lead to parabolic equations [2]. Various numerical strategies have been used to discretize this problem such as the finite element method, the finite difference method or the variational inequality method. The discontinuous Galerkin method was used to discretize Maxwell's equations. For HTS modeling, Kameni [3] used the discontinuous Galerkin method with the parabolic equations using the Interior Penalty Method for the numerical flux, which is parameter dependent. In this work, we directly work with the hyperbolic system of equations to model each material. The discontinuous Galerkin method is used to discretize the system using an upwind flux for the numerical flux. The discontinuous Galerkin method can naturally handle the discontinuity between the different materials. Numerical studies such as the linear ramping moving front problem, the modeling of an HTS-normal conductor wires and bulk surrounded by air problems will be performed. References: [1] F. Grilli, E. Pardo, A. Stenvall, N. Nguyen, W. Yuan and F. Gomory. Computation of losses in HTS under the action of varying magnetic fields and currents. IEEE Transactions on Applied Superconductivity, 24 (1) (2014) 78-110. [2] F. Grilli. Numerical modeling of HTS Applications. IEEE Transactions on Applied Superconductivity, 26 (3) (2016) 1-8. [3] A. Kameni, J. Lambrechts, J.-F. Remacle, S. Mezani, F. Bouillault and C. Geuzaine. Discontinuous galerkin method for computing induced fields in superconducting materials. IEEE Transactions on Magnetics, 48 (2) (2012) 591-594.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Scalable Generic Mesh Data Structure for Multicore Architecture

Author(s): *Nicolas Le Goff, Franck Ledoux, *CEA, France*.

Many mesh generation and adaptation algorithms are known as irregular problems, which are difficult to parallelize in a multi-threaded environment. In many cases, a key issue is to ensure the consistency of the mesh representation while avoiding deadlock and livelock situations. In order to provide an "easy" way to write meshing algorithms on multicore architecture, we rely on the Bulk-Synchronous Parallelism (BSP) model and a threadsafe mesh data structure. By adopting a BSP, parallel regions are gathered in steps where data consistency must then be ensured at the beginning and the end of each step. In our mesh data structure, a basic set of operations such as mesh entity creation and destruction is designed with threadsafe properties, while data races still have to be managed by the developer. The proposed data structure extends GMDS [1], a C++ Generic Mesh Data Structure that allows the developer to select the entities and connectivities his algorithm requires on-the-fly. It can represent any kind of unstructured surfacic and volumic meshes and provides two main kinds of representations: incidence graphs, where cells (vertices, edges, faces, regions) and useful connectivities (faces to vertices for instances) are explicitly stored; and combinatorial maps [2], where cells and connectivities are implicitly known through an algebraic structure made of a set of atomic entities, the darts D, and functions defined on D. Each representation has its own drawbacks and benefits. It is useful to have both available depending on our algorithms' requirements. In order to provide a multi-threaded implementation of such mesh representations, we rely on the Kokkos [3] programming model and its containers. Kokkos containers are used as low-level containers for both mesh representations and the BSP model gives us a canvas to write algorithms safely. Example meshing algorithms were implemented upon it to illustrate how it can be used and performance and scalability were measured on the Haswell processor as well as the Xeon Phi manycore architecture. [1] F. Ledoux, J.-C. Weill, Y. Bertrand GMDS: a Generic Mesh Data Structure. 17th International Meshing Roundtable (2008). [2] P. Lienhardt, N-dimensional generalized combinatorial maps and cellular quasi-manifolds. International Journal of Computational Geometry and Applications (1994). [3] https://github.com/kokkos.

14th U.S. National Congress on Computational Mechanics
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Title: A Frame-Guided Quadrilateral Mesh Generation Algorithm for CAD Models

Author(s): *Franck Ledoux, *CEA, DAM, DIF, France*; Katherine Lewis, Walt Nissen, *Lawrence Livermore National Laboratory, P.O. Box 808, L-488, Livermore, CA* .

For many years, surface mesh generation has been studied in numerical simulation and computer graphics communities but with different purposes. In numerical simulation, algorithms mainly focus on CAD models where curves are already meshed and target edge size and metrics are provided. In computer graphics, most of the studied models are smooth shapes and huge efforts have been done to define atlases of parametrizations, where regular quad meshes can be extracted. In this work, we use techniques coming from the computer graphics community to solve usual issues met in numerical simulation. Considering CAD models, where a set C of sharp curves is already meshed, we adapt different well-known algorithms to build the following pipeline: 1. Starting from a triangular mesh T of the CAD model boundary, a discrete frame field F is defined on T without building any surface parametrization [1]. Frames are assigned to vertices of T and they give local directions the quad mesh must follow. 2. A set of grid-aligned points P is then built from F while preserving user-defined edge constraints on C [2]. Points are grid-aligned almost everywhere but in the F singularities' vicinity. 3. Good quality quadrilateral elements are built from P directly using a direct pattern recognition algorithm. Unlike traditional approaches, this algorithms acts in the physical space and not in the parametric space [3]. 4. Remaining voids are detected and filled in using a simple triangulation algorithm before applying a blossom (?) algorithm to get a full quad mesh. The different steps of this pipeline were used to mesh several CAD models with different edge size constraints. Benefits and drawbacks of the approach are shown. [1] Practical 3D frame field generation. N. Ray, D. Sokolov and B. Lévy. ACM Transactions on Graphics (TOG), vol. 35(6), 2016. [2] Hexahedral-Dominant Meshing. D. Sokolov, N. Ray, L. untereiner and B. Lévy. ACM Transactions on Graphics (TOG), vol. 35(5), 2016. [3] Qex: Robust Quad Mesh Extraction. H.-C. Ebke, D. Bommes, M. Campen and L. Cobalt, ACM Transactions on Graphics (TOG), proceedings of SIGGRAPH Asia, pp.168:1--168:10, 2013.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Hydraulic Fracturing in Porous Media Using Phase Field Approach

Author(s): *Sanghyun Lee, Sogo Shiozawa, Mary Wheeler, *University of Texas at Austin*; Baehyun Min, *Ewha Womans University*.

Numerical simulation of hydraulic fracturing in porous media is one of the most challenging applications in petroleum, mechanical, and environmental engineering due to its complicated process involving flow-mechanics coupling as well as heterogeneous rock properties and fracture interaction. This talk will present phase field modeling approach for fluid-filled fracture propagation in poroelastic media and its applications. Here lower-dimensional fracture surface is approximated by using the phase field function. The two-field displacement phase-field system solves fully-coupled constrained minimization problem due to the crack irreversibility. This constrained optimization problem is handled by using active set strategy. The pressure is obtained by using a diffraction equation where the phase-field variable serves as an indicator function that distinguishes between the fracture and the reservoir. Then the above system is coupled via a fixed-stress iteration. In this study, we demonstrate the capabilities and applicabilities of the approach by simulating the interaction of hydraulic fractures and pre-existing fractures, fracture height growth at a layer interface with different mechanical properties and horizontal stresses, and the optimizing technique for the well and fracture (perforation) spacing for hydraulic fracture initiation to maximize the production. This is a joint work with Baehyun Min, Sogo Shiozawa, and Mary F Wheeler.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: New High-Order Methods Using Gaussian Processes for CFD

Author(s): *Dongwook Lee, *UC Santa Cruz*.

We present an entirely new class of high-order numerical algorithms for computational fluid dynamics. The new method is based on the Gaussian Processes (GP) modeling that generalizes the Gaussian probability distribution. Our approach is to adapt the idea of the GP prediction technique which utilizes the covariance kernel functions, and use it to reconstruct a high-order approximations for computational simulations. We propose the GP high-order method as a new numerical high-order formulation, alternative to the conventional polynomial-based approaches.

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Title: Polyhedral Elements Using an Edge-Based Smoothed Finite Element Method for Nearly Incompressible Material

Author(s): *Chan Lee, *Agency for Defense Development*; Hobeom Kim, Seyoung Im, *Korea Advanced Institute of Science and Technology*; Jungdo Kim, *Korea Aerospace Research Institute*.

The polyhedral elements by means of the edge-based smoothed finite element method are proposed within the framework of linear and nonlinear elasticity for nearly incompressible material. The polyhedral elements are allowed to have an arbitrary number of nodes or faces, and so retain a good geometric adaptability. The strain smoothing technique and implicit shape functions based on the linear point interpolation makes the element formulation simple and straightforward. In order to overcome the volumetric locking problem, a smoothing domain-based selective smoothed finite element method scheme and a three-field mixed cell-based smoothed finite element method with nodal cells were developed. Several numerical examples within the framework of linear and nonlinear elasticity demonstrate the accuracy and convergence behavior. The proposed schemes provide good solutions without non-physical hourglass modes.

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Title: Ab Initio Study of Interfacial Magnetoelectric Effect in Oxide Superlattice

Author(s): *Jaekwang Lee, *Pusan National University*.

Using the first-principles density functional calculations, we have investigated the magnetoelectric coupling effect in the Fe/PbTiO3/Fe superlattices by varying the number of ferroelectric PbTiO3 (PTO)layers. We find that the change of Fe magnetization is electrically tunable, linearly depending on the depolarizing field, and occurs very near the Fe/PTO/Fe interface region. The maximal magnetoelectric coupling constant is calculated to be about 4×10−10 G cm2/V. Such a remarkable coupling coefficient is quite similar order of magnitude as that recently experimentally reported from Co (7nm)/Pb(Zr,Ti)O3. We thus expect that these superlattices consisting of alternating layers of a ferromagnetic metal and a ferroelectric insulator will be promising candidates to exhibit a strong magnetoelectric coupling which stems from the simultaneous braking of the time-reversal and spatial-inversion symmetries at their interface.

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Title: Verification and Validation of Thermo-Mechanical Shock Modeling of High Energy Ball Milled Materials with Uncertainty Quantification

Author(s): *Sangmin Lee, Waad Subber, Alberto Salvadori, Karel Matous, *University of Notre Dame*.

High energy ball milling (HEBM) is a process that leads to a material with unique chemo-thermo-mechanical properties. The resulting composite from HEBM can chemically react during impact due to the complex shock wave interactions. Predicting behavior of such a complex material system is challenging because the impact test involves difficult multiphysics transient problems including: large deformations and strain rates, plasticity, chemical reactions, and heat generation. In this study, a numerically verified and experimentally validated finite element (FE) solver is developed based on the three field mixed method to incorporate the sophisticated poro-visco plastic constitutive models. The FE solver is generalized and capable of solving fully coupled multiscale and multiphysics problems such as the momentum, energy, and chemical equations. Furthermore, the solver is highly scalable in high performance computing (HPC) environments and thus allowing very demanding uncertainty quantification studies to be performed computationally. The numerical solution is verified using unit test problem and the method of manufactured solutions (MMS). The validation is performed against the reverse Taylor impact experiment which can characterize dynamic response at high strain rates. Additionally, Bayesian calibration is used to define complex slip-stick boundary conditions. Finally, results of the uncertainty quantification for the numerical simulation show good agreement with co-designed experiments. The study of several quantities of interest yields the confidence intervals for co-designing future experiments and improving numerical models.

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Title: Dynamic Tumor Growth Modeling with New Vessel Formation and Drug Delivery

Author(s): *Tae-Rin Lee, Sung Sic Yoo, *Seoul National University*.

In this talk, an integrated tumor growth model is suggested to study various correlations among new vessel formation (angiogenesis), oxygeon level and active tumor region. Unlike conventional methods for predicting endothelial cell growth and movement, we introduce a non-lattice angiogenesis model based on VEGF (vascular endothelial growth factor) gradient. The proposed model integrates tumor growth, VEGF secretion, angiogenesis, oxygen diffusion and blood flow. Furthermore, vessel bifurcation and anastomosis are considered in the dynamic vessel growth of tumor microvascular networks in 3D space. For the validation, several numerical studies are performed in a virtual system similar to real tumor microenvironment. In addition, as a practical application, drug delivery scenarios are coupled with the proposed model. The cellular interaction between tumor growth and drug delivery is quantitatively calculated in the tumor microenvironment.

14th U.S. National Congress on Computational Mechanics
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Title: Reduced Order Models and Optimization of Elastomer Damping Devices

Author(s): *Antoine Legay, Jean-François Deü, Benjamin Morin, Sylvain Burri, *LMSSC, CNAM, Paris, France*.

Due to their damping properties, elastomer materials are commonly used in the industry to achieve anti-vibration junctions between mechanical subsystems. These links are usually made of various materials (metallic, composites and elastomers). Moreover, there geometries may be optimized in order to fulfill the needs of the specific targeted application. But in order to predict the dynamic behavior of these junctions in their environment, efficient numerical dynamic models have to be developed. These models should take into account the viscoelastic behavior of the elastomer and the material and geometric nonlinearity. The objective of this work is thus to develop methods to optimize flexible damping devices made of elastomer as well as to build efficient models for the prediction of their dynamic behavior. Firstly, a three-dimensional finite element nonlinear code using hyper-viscoelasticity constitutive relations is developed for the numerical modeling of the elastomer junctions. Secondly, a topological optimization [1] of the damping device is achieved in order to find the best geometry shape. Thirdly, a reduced order model is developed. It is based on a component mode synthesis method adapted to highly damped structures by using a multi-model approach [2]. The final reduced element representing the junction is obtained by a dynamic condensation on the external rigid faces in contact with the sub-structures for a total of 12 dofs (6 dofs per face) [3]. The presented application is a junction used to damp the transmitting vibrations from a vibrating base to a support of a sensible device such as an on-board camera (in an UAV or in a plane for instance). [1] M.P. Bendsoe, O. Sigmund. Topology Optimization. Theory, Methods, and Applications. Springer, 2004. [2] L. Rouleau, J.-F. Deü, A. Legay. A comparison of model reduction techniques based on modal projection for structures with frequency-dependent damping. Mechanical Systems and Signal Processing, 90, 110–125, 2017. [3] A. Legay, J.-F. Deü, B. Morin. Reduced order models for dynamic behavior of prestressed elastomer damping devices. Proceedings of the VII European Congress on Computational Methods in Applied Sciences and Engineering, the ECCOMAS Congress 2016, Hersonissos, Crete, Greece, June 5-10, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: A Posteriori Error Estimation for Multiscale Computations Based on MsFEM

Author(s): *Frederic Legoll, *ENPC and INRIA*; Ludovic Chamoin, *ENS Cachan*.

The Multiscale Finite Element Method (MsFEM) is a Finite Element type approach for multiscale PDEs, where the basis functions used to generate the approximation space are precomputed and are specifically adapted to the problem at hand. The computation is performed in a two-stage procedure: (i) a offline stage, in which local basis functions are computed, and (ii) a online stage, in which the global problem is solved using an inexpensive Galerkin approximation. Several variants of the approach have been proposed and a priori error estimates have been established. As for any numerical method, a crucial issue is to control the accuracy of the numerical solution provided by the MsFEM approach. In this work, we develop an a posteriori error estimate and the associated adaptive procedure. The estimate is based on the concept of Constitutive Relation Error (CRE), which we extend to the multiscale framework. We introduce a guaranteed and fully computable a posteriori error estimate, both for the global error and for the error on quantities of interest, using adjoint-based techniques. We discuss the accuracy of such estimates and show how they can be used to efficiently drive an adaptive discretization. Time permitting, we also investigate the additional use of model reduction techniques (such as the Proper Generalized Decomposition (PGD)) within the MsFEM approach in order to further decrease the computational costs. Joint work with L. Chamoin.

14th U.S. National Congress on Computational Mechanics
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Title: Using Peridynamics to Model Biological Materials

Author(s): *Emma Lejeune, Christian Linder, *Stanford University*.

A better understanding of tumor growth and tumor response to intervention has the potential to guide clinical decision making. In particular, computational modeling can be used to better understand how processes that are well defined only on the cellular and sub-cellular scales manifest on the tissue scale, and can be used to predict how a tumor will progress and interact with surrounding healthy tissue. Though much work has been done in this field, many open questions remain. Here we show how the dual-horizon peridynamic framework can be adapted to model biological materials, particularly tumors, and discuss why peridynamics is well equipped to handle many of the challenges associated with modeling biological materials. Then, we discuss recent applications of this modeling technique, where we investigate the influence of cellular scale division angle during cell proliferation on macroscale tissue growth and the influence of cellular scale cell death mechanisms on macroscale tissue shrinkage. This initial work shows that the peridynamic framework is a useful tool for modeling biological tissue, particularly tumors. [1] Lejeune, E., & Linder, C. (2017). Modeling tumor growth with peridynamics. Biomechanics and Modeling in Mechanobiology, 1-17. [2] Lejeune, E., & Linder, C. (2017). Quantifying the relationship between cell division angle and morphogenesis through computational modeling. Journal of Theoretical Biology, 418, 1-7.

14th U.S. National Congress on Computational Mechanics
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Title: A New Paradigm for the Numerical Approximation of Sign-Changing Problems

Author(s): Assyr Abdulle, *Simon Lemaire, *EPFL (Lausanne, Switzerland)*.

We consider a diffusion problem with a diffusivity coefficient that changes sign in the domain. This kind of problems arises, e.g., in the modeling of the interface between a dielectric and a (negative) metamaterial. Recently, in [1], the homogenization of periodic structures made up of negative inclusions in a positive matrix has been considered, and a (partial) theory has been developed. However, performing numerics for these configurations requires to solve sign-changing cell problems. The numerical approximation of sign-changing equations has been investigated in [2] but the approach therein is based on restrictive meshing assumptions, and does not apply to all interesting practical cases. We introduce a new paradigm for the approximation of sign-changing problems, that is based on optimization. Our approach [3] does not rely on any meshing assumption and applies without limitations. With such a numerical method, it is possible to investigate the definiteness of the effective coefficients derived in [1] for various geometrical configurations. [1] R. Bunoiu and K. Ramdani. Homogenization of materials with sign changing coefficients. Communications in Mathematical Sciences, 14(4):1137-1154, 2016. [2] L. Chesnel and P. Ciarlet Jr. T-coercivity and continuous Galerkin methods: application to transmission problems with sign-changing coefficients. Numer. Math., 124:1–29, 2013. [3] A. Abdulle, M. E. Huber, and S. Lemaire. An optimization-based numerical method for diffusion problems with sign-changing coefficients. Accepted in C. R. Acad. Sci. Paris, Série I, to appear. Available at hal-01354092v2.

14th U.S. National Congress on Computational Mechanics
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Title: High-Fidelity Simulation of Brittle Fracture Problems with Universal Meshes

Author(s): *Adrian Lew, *Stanford University*.

We describe our approach to computing fracture propagation paths in two-dimensions, based on: (a) a method to compute arbitrary high-order approximation of linear elastic solutions around a crack, and (b) a method to extract the stress intensity factors from the solutions which converges with double the rate of convergence of the stresses. As a result, coarser meshes can be used to extract values of the stress intensity factors at each crack propagation step with high accuracy. In particular, when we combine these tools with a background Universal Mesh, we are able to propagate cracks by essetially using the same background mesh for the entire path. Additionally, the crack paths are converged, and hence are independent of the background mesh adopted for the calculations. In the presentation I will introduce the notion of a Universal Mesh and the high-order method to compute the stress intensity factors, and demonstrate their use in the propagation of a thermally driven crack and a hydraulic fracture. This work will show joint contributions from: Maurizio Chiaramonte, Ramsharan Rangarajan, Benjamin Grossman-Ponemon, Yongxing Shen, Leon Keer, and Michael Hunsweck.

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Title: The Shifted Boundary Method: A New Approach to Embedded Boundary Computations

Author(s): Guglielmo Scovazzi, Alex Main, Nabil Atallah, Ting Song, *Kangan Li, *Duke University*.

Embedded boundary methods obviate the need for continual re-meshing in many applications involving rapid prototyping and design. Unfortunately, many finite element embedded boundary methods for incompressible flow are also difficult to implement due to the need to perform complex cell cutting operations at boundaries, and the consequences that these operations may have on the overall conditioning of the ensuing algebraic problems. We present a new, stable, and simple embedded boundary method, which we call “shifted boundary method” (SBM), that eliminates the need to perform cell cutting. Boundary conditions are imposed on a surrogate discrete boundary, lying on the interior of the true boundary interface. We then construct appropriate field extension operators, with the purpose of preserving accuracy when imposing the boundary conditions. We demonstrate the SBM on large-scale incompressible flow problems, multiphase flow problems, solid mechanics problems, and shallow water flow problems.

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Title: Nonlocal Heat Conduction Models in Nano-Scale Materials: First Principle Derivations and Local Approximations

Author(s): *Xiantao Li, *Pennsylvania State University*.

This talk will present the derivation of nonlocal heat conduction models to capture the non-Fourier heat conduction in nanoscale materials. We start with a full atomistic or quantum mechanical model, and derive a constitutive relation for the heat flux. In addition, we discuss local approximations, in the form of high order partial differential equations. Comparisons will be made with existing empirical models.

14th U.S. National Congress on Computational Mechanics
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Title: Soft Matter Modeling and Simulation of Mechanotransduction of Cells

Author(s): *Shaofan Li, *University of California* .

In this presentation, we shall discuss our recent work on soft matter modeling and multiscale simulations of the contact and adhesion of cells with the extracellular substrate. In particular, we are interested in how extracellular mechanical properties will affect such contact and adhesion process and how these cell/substrate interaction translate into mechanical signals coming back into the cell that manifest through its deformation, configuration, as well as molecular conformation changes. In order to understand overall mechanical process of cell contact and adhesion, and to explain the possible mechanotransduction mechanism, we have developed a three-dimensional soft-matter cell models that use the liquid-crystal or liquid-crystal elastomer models to represent the overall constitutive relations of the cell in order to simulate their response to extra-cellular stimulus. In this work, we have systematically developed a three-dimensional cell model by treating the cell as a special type of soft matters. A multi-component three-dimensional cell model with a coarse grained adhesion potential has been formulated and implemented in numerical simulations. In our model, the utmost layer is a layer of liquid crystal, and the inner cell is modeled as a hyperelastic core. The extra-cellular matrix is modeled as a substrate of hyperelastic block or a liquid crystal polymer layer. To accurately model the contact and adhesion of between the substrate and stem cells, the state-of-art numerical modeling techniques are adopted in our modeling and simulation procedures such as the multiscale moving contact line theory, etc. Our simulations have shown some remarkable features of cell contact and adhesion that have never been observed before, such as (1) cell spreading induced by combination of adhesive force and surface tension and its sensitivity to substrate rigidities; (2) cell shape evolution and the evolution of cell mesogen director orientation distribution, which is an indicator of overall myosin structure of the cell, and (3) evolution of traction force between the cell and substrate.

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Title: Recent Progress on DG Methods for Maxwell's Equations in Complex Media

Author(s): Yunqing Huang, Wei Yang, *Xiangtan University*; *Jichun Li, *University of Nevada Las Vegas*.

Inspired by the successful construction of metamaterials in 2000 and its many interesting potential applications (such as invisibility cloak and subwavelength imaging), we developed some DG methods for simulating wave propagation in metamaterials in recent years [1,2,3]. In this talk, we will present a review of our past works on DG methods. More specifically, we like to talk about the posteriori error estimate obtained for the IPDG method developed for time-dependent integral-differential Maxwell's equations in cold plasma, and the edge element method for time-dependent Maxwell's equations. Application of a posteriori error estimator to invisibility cloak will be demonstrated. Some open issues will be mentioned. [1] J. Li and Y. Huang, Time-Domain Finite Element Methods for Maxwell's Equations in Metamaterials, Springer Series in Computational Mathematics, vol.43, Springer, 2013. [2] J. Li, Posteriori error estimation for an interiori penalty discontinuous Galerkin method for Maxwell's equations in cold plasma, Adv. Appl. Math. Mech. 1 (2009) 107--124. [3] J. Li, Y. Huang and W. Yang, An adaptive edge finite element method for electromagnetic cloaking simulation, Journal of Computational Physics 249 (2013) 216–232.

14th U.S. National Congress on Computational Mechanics
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Title: A New Multigrid Method for Saddle Point Problems

Author(s): *Hengguang Li, *Wayne State University*.

We develop new multigrid methods for a class of saddle point problems that include the Stokes system in fluid flow and the Lamé system in linear elasticity as special cases. The new smoothers in the multigrid methods involve optimal preconditioners for the discrete Laplace operator. We prove uniform convergence of the W-cycle algorithm in the energy norm and present numerical results for W-cycle and V-cycle algorithms. We also discuss the extension of our methods to the nonsymmetric Oseen system.

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Title: Atomistic-to-Continuum Influenced Consistent Coupling of Nonlocal Diffusion Problems

Author(s): *Xingjie Li, *UNC at Charlotte*; Jianfeng Lu, *Duke University*; Xiaochuan Tian, Qiang Du, *Columbia University*.

Nonlocal models have been developed and have received a lot of attention in recent years to model systems with important scientific and engineering applications. While it is established that the nonlocal formulations can often provide more accurate descriptions of the systems, the nonlocality also increases the computational cost compared to conventional models based on PDEs. In this talk, I will introduce a recently developed self-adjoint, consistent, and stable coupling strategy for nonlocal diffusion models, inspired by the quasinonlocal atomistic-to-continuum method for crystalline solids. The proposed coupling model is coercive with respect to the energy norms induced by the nonlocal diffusion kernels as well as the L2 norm, and it satisfies the maximum principle. A finite difference approximation is used to discretize the coupled system, which inherits the property from the continuous formulation. Furthermore, we design a numerical example which shows the discrepancy between the fully nonlocal and fully local diffusions, whereas the result of the coupled diffusion agrees with that of the fully nonlocal diffusion.

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Title: Computational Design of Hierarchical Structures for Crashworthiness Criteria

Author(s): Guangyong Sun, Jianguang Fang, *Qing Li, *The University of Sydney*.

As a class of widely observed materials in nature, hierarchical microstructures may be of superior mechanical properties. In this study, we incorporate the concept of hierarchy into honeycomb structures for enhancing their crashworthiness performance. Hierarchical honeycombs are constructed by replacing every vertex of a regular hexagonal network with a smaller hexagon topology and repeating this process for constructing fractal-appearing honeycombs with higher order of structural hierarchy. To examine the crashing characteristics, the hierarchical honeycombs with the first-order and second-order structures were investigated under an out of the cross-sectional plane loading scenario. A parametric study on structural variables were undertaken with three different apparent densities. A comparison between regular honeycombs and hierarchical honeycombs was conducted. The results showed that the out-of-plane energy absorption of the first-order hierarchical honeycombs and the second-order hierarchical honeycombs with a certain structural parameters have better overall performance. Further, the specific energy absorptions (SEA) of the first-order hierarchy and the second-order hierarchy were improved about 65.9% and 185.7%, respectively. Moreover, their corresponding peak forces do not increase compared with the regular honeycomb under the same density, indicating that hierarchical honeycombs can be an ideal lightweight structure for designing crashworthy structures. Reference GY Sun, H Jiang, JG Fang, GY Li, Q Li. Crashworthiness of vertex based hierarchical honeycombs in out-of-plane impact. Materials & Design 110 (2016) 705-719.

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Title: The Cell Differentiation Model for Dental Implants

Author(s): *Ming Jun Li, Nien-Ti Tsou, *National Chiao Tung University*.

The dental implant is the common device to assist the recovery of the teeth. However, it often has poor primary stability which causes the failure of the surgery. One of the main reasons is the loosening of the dental implant in the early stage of healing callus. In this study, a peri-bone healing model of the dental implant under the immediate loading is developed and used to predict the level of the osseointegration between the considered implants and the bones, giving the evaluation of the primary stability and the dental implants. The porous finite elements with both solid- and fluid-phase stimuli are used to simulate the healing process of the bone. The diffusion of stem cells is also considered for the dynamic simulation. The differentiation, growth, and resorption can be determined based on the criteria reported by Lacroix et al[1]. The model is applied to study several implants with an axisymmetric geometry. Many features of the osseointegration are revealed by the model, having good agreement with those observed in the experimental results. For example, the bone resorption between threads due to the stress shielding effect; the fibrous layers form in the callus region. The current model is expected to provide design guidelines for the dental implants with arbitrary shapes . [1] Lacroix, D., Prendergast, P.J., 2002. A mechano-regulation model for tissue differentiation during fracture healing: analysis of gap size and loading. Journal of Biomechanics 35, 1163–1171.

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Title: Topology Optimization of Elastoplastic Structures under Cyclic Loads

Author(s): *Lei Li, Guodong Zhang, Kapil Khandewal, *University of Notre Dame*.

Topology optimization of elastoplastic structures is an important research topic that had received increasing interests in recent years. Unlike the linear and nonlinear elastic problems, elastoplastic problem is path-dependent, indicating that the structural response and the corresponding response sensitivities are history dependent. Due to this irreversibility of the plastic deformation process, an important application of elastoplastic topology optimization is the design of energy absorbing elastoplastic structures that can dissipate energy as plastic work. Previous studies on elastoplastic topology optimization mainly focused on monotonic loads and isotropic hardening models. Up to now, there is no study that explicitly investigated elastoplastic topology optimization under cyclic loading conditions, which are important in many practical applications. For example, one such application includes design of passive protective devices that employ metallic yielding to dissipate energy under seismic excitations. Such protective devices usually dissipate energy via plastic work under a few but large loading cycles. In this scenario, the cyclic loading history applied to the structure is critical and has a significant influence on the final optimized topologies, which should be appropriately considered in the design phase. In this study, we propose a novel elastoplastic topology optimization methodology with the consideration of cyclic loading scenario. To simulate the well-known Bauschinger effect under cyclic loads, the Prager linear kinematic hardening rule and the Armstrong-Frederick nonlinear kinematic hardening rule are incorporated together with the von Mises plasticity [1]. A consistent adjoint method is presented for the path-dependent sensitivity analysis [2]. It is shown through the presented numerical examples that the optimized designs vary under different cyclic loading patterns. More importantly, this topological difference becomes significant if the Bauschinger effect is dominating. References: [1] Chaboche JL (1989) Constitutive equations for cyclic plasticity and cyclic viscoplasticity. International Journal of Plasticity 5 (3):247-302. [2] Zhang G, Li L, Khandelwal K (2017) Topology optimization of structures with anisotropic plastic materials using enhanced assumed strain elements. Structural and Multidisciplinary Optimization, doi:101007/s00158-016-1612-1. Keywords: Topology optimization; von Mises plasticity; Cyclic loads; Kinematic hardening; Adjoint sensitivity analysis; Plastic work.

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Title: Phase-Field Modeling of Selective Laser Melting at the Powder level

Author(s): *Jiqin Li, Tai-Hsi Fan, *University of Connecticut*.

Selective laser melting and sintering of metallic, polymer, and composite powders are commonly used in additive manufacturing (AM) for building geometrically complicated parts that are otherwise difficult to manufacture by conventional methods. However, the surface quality of AM-produced parts is often inferior to conventionally machined parts. This shortfall hinders the AM applications on producing high-end products especially for aerospace and biomedical applications. To overcome this difficulty and advance the laser-based AM technology, better understanding of the underlying thermal-fluid processes at the powder level is necessary to provide quantitative information and to optimize the relevant manufacturing processes. AM processes often cover melting, vaporization, re-solidification, and/or sintering at the powder level, and these processes are further complicated by dynamic powder-powder interactions, interfacial transport, a broad range of temperature-dependent thermophysical properties, and the fully coupled fluid flow and multi-mode heat transfer (including conduction, convection, and thermal radiation) induced by a spot laser heating. Here we focus on multiphase thermal fluid simulation using phase-field approach to characterize powder melting and thermal capillary flow dynamics of pure metal powder(s) with a simplified 2D configuration. Pure titanium power(s) with diameter about tens of microns are heated by a moving Gaussian laser beam. The governing system involving liquid-solid phase transition, fluid flow of the molten metal, and the thermal capillary effect are formulated by the entropy-based phase-field framework. Even though evaporation of the liquid metal and the dynamics of the surrounding gas phase are neglected, the system results in about ten dimensionless groups in the theoretical analysis for basic characterization. The simulation resolves the phase transition dynamics including moving solid-liquid interface and transient temperature distribution during the heating process. The role of Korteweg stress in the thermal capillary flow and enhanced heat transfer will be discussed in detail. The numerical model can be extended for further investigation of dynamic powder-powder interactions as a critical step in advancing the design, control, and optimization of surface quality of AM products.

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Title: Abnormal Vascular Dynamics of Nanoworms within Blood Flow

Author(s): *Ying Li, Huilin Ye, *University of Connecticut*.

Through nanomedicine, game-changing methods are emerging to deliver drug molecules directly to diseased areas. One of the most promising of these is the targeted delivery of drugs and imaging agents via drug carrier-based platforms. Such drug delivery systems can now be synthesized from a wide range of different materials, made in a number of different shapes, and coated with an array of different organic molecules, including ligands. If optimized, these systems can enhance the efficacy and specificity of delivery compared with those of non-targeted systems. Emerging integrated multiscale experiments, models and simulations have opened the door for endless medical applications. Current bottlenecks in design of the drug-carrying particles are the lack of knowledge about the dispersion of these particles in the microvasculature. To provide fundamental insights into the blood circulation behaviors of nanoparticles, mathematical simulations have been performed to understand the transport behaviors of nanoparticles in the presence of red blood cells (RBCs). Under the normal physiological conditions (shear rate 100 s-1 and hematocrit 30%), the deformable RBCs are more concentrated within the core region of blood vessel, leaving few micrometers of 'cell-free-layer' near the vessel wall. The injected rigid spheres are pushed into the cell-free-layer due to their repulsive interactions with the concentered RBCs in the core region. Such a margination effect has been observed for white blood cells and platelets. When the rigid spheres are substituted by the rigid nanoworms, a similar phenomenon has been observed. However, the margination of the rigid nanoworms is slower than the spheres, likely due to their slender shapes. The most interesting phenomenon has been observed for soft nanoworms. These flexible nanoworms can easily accommodate their deformations with the deformed RBCs in the blood flow. Therefore, these flexible nanoworms can circulate with RBCs in the blood flow, with negligible margination within the simulation time. From these simulation results, the shape (or aspect ratio) and stiffness (flexibility) are found to play important roles in design of drug carriers with high efficacy.

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Title: Molecular Dynamics Simulations of a Porous Nano-Fluidic Desalination Device

Author(s): *tiange li, shaofan li, *University of California, Berkeley*.

A porous nano-fluidic desalination device, a rotating carbon nanotube membrane filter with conical frustum geometry, is designed for the reverse osmosis desalination that can turn salt water into fresh water. We have used molecular dynamics to model and to simulate the proposed graphene membrane nano-fluidic device. Molecular dynamics simulations are performed at different pressures to simulate the proposed carbon nanotube (CNT) membrane filters with varying pore diameters (2.8–5.7 Å). The results have shown that the fresh water permeation rate depends on the angular velocity of the rotating model, from 1.75 rad/ns to 175 rad/ns, and the number of pores, from 1 to 35, on the CNT wall. In particular, the simulation results show that the seawater can continuously flow through the proposed nano-fluidic device and form a loop without additional external pressure, because the component of the support force from CNT wall to water and ions makes water and ions move towards one end of the conical frustum geometry model. By selecting an optimized pore size, angular velocity and number of pores, we also examined the desalination efficiency of the proposed nanoscale fluidic device, and we have compared the overall efficiency of this model with other methods. Besides the application to seawater desalination, the potential application of the proposed nanoscale separation model is multitude. The proposed nano-fluidic device can be applied to other areas by changing the pore size on CNT wall or changing the angular velocity to create different types of nano-channels for different purposes, such as separation of isotopes of Uranium, separation of virus from blood cells, and separation of much bigger organic molecules.

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Title: A Phase-Aware Meshfree Framework for Dynamic Behavior of Materials under Extreme Thermomechanical Conditions

Author(s): *Bo Li, Hao Wang, Zongyue Fan, *Case Western Reserve Univ.*.

We present a phase-aware incremental Lagrangian framework based on meshfree methods for a robust and efficient solution of materials behavior under extreme thermomechanical loading conditions. The proposed framework combines the Optimal Transportation Meshfree (OTM) method and the variational thermomechanical constitutive updates. In particular, the variational structure of dynamic systems with general internal dissipative mechanisms is discretized in time by applying the Optimal Transportation theory. Furthermore, material points and nodes are introduced for the spatial discretization of the domain. In this work, kinematic information of the system including displacement and temperature is defined at the nodes, but material local state and constitutive responses are evaluated at the material points. Meshfree shape functions, such as the Local Maximum Entropy (LME) approximation scheme, may be employed to construct the continuous incremental motion and temperature field. The deformation, temperature and internal variables are therefore obtained at the stationary of the fully discretized action. In order to solve the strongly coupled thermomechanical equations efficiently, we adopt the operator split algorithm. Specifically, at each iteration, the discretized mechanical equations are solved explicitly at the nodes with embedded implicit processes to compute the internal variables at material points assuming adiabatic conditions. The discretized thermal equations are then solved implicitly assuming mechanical equilibrium to update the temperature distribution when the thermal driving forces reach a critical value. As a consequence, the internal energy dissipation and heat transfer contribute to the local temperature change, which directly determines the materials local state including solid, liquid and gas phases. The range and scope of the presented method is demonstrated by means of two examples of application: typical hot forming processes for the fabrication of composite materials and powder bed fusion based additive manufacturing processes of metals.

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Title: A 3D Numerical Limit Analysis Approach for Strength Predictions of Cross-Laminated Timber Plates

Author(s): *Mingjing Li, Josef Füssl, Markus Lukacevic, Josef Eberhardsteiner, *TU Vienna*.

In recent years, cross-laminated timber (CLT), as an innovative wood-based product, has been increasingly used in high-performance building structures. However, due to the complexity and variety of the raw material properties, existing numerical tools for strength predictions are not sufficiently satisfying, regarding efficiency and accuracy. Since structural failure of CLT shows significant ductile behavior, limit analysis seems to be an appropriate method to obtain strength predictions in an efficient way. Thus, this contribution focuses on numerical limit analysis approaches capable of dealing with the complex material behavior of wood. This method, known as direct method, focuses directly on the time instant of failure, and therefore, has significant advantage over the traditional step-by-step iterative methods regarding computational efficiency. Within the presented concepts, two nonlinear optimization problems are to be solved, leading to a lower bound and an upper bound of the considered effective CLT strength. The 3D CLT models are discretized by tetrahedron elements, anisotropic yield functions are employed for plastic failure, and the nonlinear optimization problems are solved efficiently by second-order cone programming (SOCP). According to experimental observations, failure mechanism in CLT plates are highly localized. Thus, in the upper bound approaches velocity discontinuities were introduced between tetrahedron elements, serving as additional degrees of freedom. In that way, localized failure could be estimated more precisely and efficiently. In order to guarantee a consistent strength behavior for both interface failure as well as failure within solid elements, a mathematical transformation was applied which projected the anisotropic stress-based yield functions to traction-based yield functions, assigned to interfaces. A good agreement between numerical results and experimental data, obtained from bending tests on CLT, was obtained. Due to the high efficiency of this numerical approach, it could be extended to stochastic considerations, in which the probability distribution functions of the effective bending strength of CLT plates were derived according to the grade of wooden boards. The results may serve as basis for CLT optimization and / or support complex fracture mechanical approaches by providing information about failure mechanisms in advance.

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Title: Adaptive Stochastic Approximation for Transport Problems with Random Input Data

Author(s): *Jason Li, Assad Oberai, Onkar Sahni, *Rensselaer Polytechnic Inst.*; Eric Cyr, Eric Phipps, *Sandia Labs*.

For many transport problems of interest, the solution is a complex function of random variables (e.g., in a case of a distributed array of flow streams or jets). For such problems, an adaptive approach to construct the solution approximation is more efficient. In this work we will present an adaptive formulation based on the variational multiscale (VMS) method for stochastic PDEs with uncertain input data that include material parameters, boundary conditions, and source terms. In this approach, we employ finite elements in the physical domain and spectral approximation based on generalized polynomial chaos in the stochastic domain. The VMS method leads to an accurate solution in a coarse space while accounting for the missing/fine scales through a model term. The fine scales in the model term are approximated as the product of the strong-form residual and a stochastic stabilization parameter. This relatively inexpensive approximation for the fine scales is also used to estimate the error in the numerical solution in a local/element-wise fashion and to drive adaptivity in the physical and spectral approximations. The performance of this adaptive strategy is benchmarked on advective-diffusive transport problems.

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Title: Unstructured and Anisotropic Adaptivity for Complex Stochastic Problems

Author(s): Onkar Sahni, *Jason Li, Alvin Zhang, *Rensselaer Polytechnic Inst.*.

Adaptive approaches have been shown to be very effective in performing reliable predictions for complex problems. Specifically unstructured adaptive methods have resulted in significant savings in the computational cost for such problems. In addition, solution features for many problems exhibit a local directional behavior that must be efficiently addressed using a locally anisotropic discretization. In this work, we will present some ideas on formulation and application of unstructured and anisotropic adaptivity in the context of stochastic PDEs with uncertain or random input data that include material parameters, boundary conditions, and source terms. We will present results for multi-physics transport problems. Note: This talk is dedicated to my mentor, colleague and friend Prof. Mark Shephard on his 65th birthday.

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Title: A Novel Macro/Micro-Structure Optimization Design Method for Additive Manufactured Structures

Author(s): *Zhao Libin, *School of Astronautics, Beihan University*.

Additive manufacturing (AM) technique has greatly open up the freedom of the topology optimization and makes it possible to design and optimize in both macro and micro levels and create structures with brilliant mechanical properties and other advantages. A novel macro/micro-structure optimization design method was proposed in this paper to further homogenize the stress distribution and reduce the weight of the structures manufactured by AM techniques. In the macro-structure level, based on the notion of the Evolutionary Structural Optimization (ESO) method, stiffness of the units of the primary structures was adjusted in an iteration loop. Elastic modulus of the low-stress units was degenerated and high-stress units were remained in each cycle. After iteration, the structure with the optimal loading path was obtained. In the micro-structure level, the lattice cells were utilized to replace part of relatively low-stress units in the structures according to the substitution criterion established in the paper. Based on the thought of equivalent substitution, the radius of strut of the lattice cell was arranged according to the elastic modulus of the units. The hollow lattice structure with optimal loading path was gained. Besides, the comparisons of the mechanical properties between the hollow lattice structure and the structure from the traditional ESO method were also provided in the paper. Keywords: Evolutionary Structural Optimization; lattice structure; equivalent substitution. Affiliations: 1. School of Astronautics, Beihang University, Beijing 100191, China; 2. Aero-polytechnology Establishment, Aviation Industry Corporation of China, Beijing 100191, China.

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Title: Direct and Simultaneous Extraction of Vector Traction-Separation Relations for Interfaces

Author(s): *Kenneth Liechti, Rui Huang, *University of Texas Austin*; Chenglin Wu , *Missouri University of Science and Technology*.

Traction-separation relations can be used to represent the interactions between two surfaces during separation. In the past, characterizing these interactions, particularly under mixed-mode conditions has been tedious. In this paper, a direct method is proposed to simultaneously determine the normal and shear components of traction-separation relations at any mode-mix, based solely on measurements of the crack length, load and load-line displacement and rotation of each adherend in a laminated beam configuration. An analysis of the end loaded split (ELS) and end notched flexure (ENF) configurations that accounts for the normal and shear tractions between two layers is used to establish how the differential equations for the normal and shear separations can be decoupled, even under the mixed-mode conditions provided by these configurations. Interestingly, the decoupled configurations do not hinder the ability to provide a range of mixed-mode conditions via asymmetries in the mechanical properties and thickness of the layers. A series of experiments were conducted to extract the vector traction-separation relations between silicon and epoxy over a wide range of mixed-mode conditions for positive and negative shear. A custom-built loading device was developed to provide the measurements alluded to above. Since the vector traction-separation relations are extracted in a direct manner with no a priori assumptions as to their form, it was possible to examine the applicability of potential versus non potential representations of mixed-mode traction-separation relations for this interface.

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Title: Developing Physically-Based Three Dimensional Polycrystalline Microstructures

Author(s): *Hojun Lim, Fadi Abdeljawad, Steve Owen, James Foulk, *Sandia National Laboratories*; Jacob Gruber, Garritt Tucker, *Drexel University*.

Concurrent trends in various technologies are moving towards component miniaturization and increased realism in predictive simulations. This leads to a necessity for microstructure-aware analysis capabilities for a variety of applications. In this work, novel techniques to create physically-based atomistic and continuum-scale realizations of polycrystalline aggregates using phase field grain growth model are discussed. The proposed meshing techniques are used in molecular dynamics (MD) and crystal plasticity finite element (CP-FE) simulations of polycrystalline metals and compared with conventional approaches using Voronoi tessellation and voxelated representation of microstructures. While little difference is exhibited in the macroscale mechanical response, substantial differences in the local phenomena were observed in simulations in both length scales. Furthermore, this framework provides a direct link between two computational models, MD and crystal plasticity, and allows simulations of polycrystalline materials with physically-based topological features.

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Title: Development of Phase-Field Models of Tumor Growth with Radiation Effects

Author(s): *Ernesto A B F Lima, Amir Shamoradi, David A Hormuth II, J Tinsley Oden, Thomas E Yankeelov, *University of Texas at Austin*; Thomas Horger, Barbara Wohlmuth, *Technical University of Munich*.

Introduction: The development of computational models that reliably predict the growth or decline of tumors in living tissue is one of the great challenges in modern predictive science. The present investigation extends the work in [1,2] to the prediction of effects of X-ray radiation applied in a murine model of glioma. New models of the decline in tumor cell proliferation due to radiation are presented and validated against MRI data. Methods: The starting point for developing plausible models for tumor growth involves first, an appeal to fundamental balance laws of physics, represented by the continuum theory of mixture, and then proceeds to the consideration of mathematical characterizations of well-known biological events that are known to promote or control the growth and decline of tumors. We propose five, thermodynamically consistent, phase-field tumor growth models, with and without mechanical deformation, that describe the evolution of tumor volume fraction fields in living tissue. The classical linear-quadratic survival-versus-dose model is used to develop mass sinks in mass balance equations for tumor cell volume fraction. We consider a new model, with a Type-II response (using the language of ecology), which is designed to mimic observed effects in rat model of glioma. The Occam Plausibility Algorithm (OPAL) [3] is used to calibrate, validate, and select models that best correspond to the observed MRI data. Results: The proposed models are able to reproduce the tumor area evolution observed during in vivo experiments. The results indicate that for the scenarios employed, with the tolerance prescribed, and for a single dose treatment plan, the new treatment term is the best model among the class considered, being select as valid by the OPAL framework (i.e. within 7% area difference from the data). Conclusion: We demonstrate that OPAL is able to assist in the selection of the best radiotherapy tumor growth model from a defined set of models. The extension of this study to different scenarios including 3D experiments and the prediction of the shape of the tumor will also be presented. Acknowledgments: The CPRIT through RR160005, the NCI through U01CA174706 and R01CA186193, the U.S. DOE Office of Science under DE-5C0009286. References: [1] Lima et al, Math Models Methods Appl Sci, 2016; 26(12): 2341-2368. [2] Hormuth II et al, Phys Biol, 2015; 12(4): 046006. [3] Farrel et al, J Comput Phys, 2015; 295(15): 189-208.

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Title: Towards Scalable AMG-Based Preconditioners for MHD and Multifluid Plasma Simulations

Author(s): *Paul Lin, *Sandia National Laboratories*; John Shadid, Edward Phillips, Jonathan Hu, Eric Cyr, Roger Pawlowski, .

Continuum modeling for plasma physics systems involves the solution of the governing partial differential equations (PDEs) describing conservation of mass, momentum, and total energy for each fluid species, along with Maxwell's equations for the electromagnetic fields. In this study we consider spatial discretization approaches based on structure-preserving finite element methods on unstructured meshes. For the solution of the discrete nonlinear system, the use of fully-coupled Newton-Krylov solution approaches can be advantageous because of their robustness for complex multiphysics problems. Block preconditioners are employed to deal with the disparate discretization for the fluid and the electromagnetic variables for the linearized systems. These techniques utilize approximate block factorization (ABF) methods and physics-based preconditioning approaches that reduce the coupled systems into a set of simplified systems to which specialized multilevel methods are applied. We examine the scaling and performance of our algebraic multigrid-based preconditioned Newton-Krylov solution approach [1-3] based on Trilinos solver library components for MHD and multifluid plasma simulations. Our focus will be on large-scale, transient plasma simulations. We present scaling results for resistive MHD and initial results for multifluid / full-Maxwell plasma test cases. References [1] P. Lin, "Improving multigrid performance for unstructured mesh drift-diffusion simulations on 147,000 cores," International Journal for Numerical Methods in Engineering, 2012, Vol. 91, pp. 971-989 [2] J. Shadid, R. Pawlowski, E. Cyr, R. Tuminaro, P. Weber and L. Chacon, "Scalable Implicit Incompressible Resistive MHD with Stabilized FE and Fully-coupled Newton-Krylov-AMG," Computer Methods in Applied Mechanics and Engineering, 2016, Vol. 304, pp. 1-25 [3] E.C. Cyr, J.N. Shadid and R.S. Tuminaro, "Teko an abstract block preconditioning capability with concrete example applications to Navier-Stokes and resistive MHD," SIAM SISC, 2016, Vol. 38, No. 5, pp. S307–S331

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Title: A Volume-Conserving Level Set Method on Unstructured Meshes Using a Control Volume Finite Element Formulation

Author(s): *Stephen Lin, Jinhui Yan, Gregory Wagner, *Northwestern University*.

The level set method is an approach for implicitly resolving interface geometry and has been widely applied to simulation of multiphase flow problems. However, many of the components of this method, such as the redistancing of the level set function to retain a signed-distance function property, become more difficult on unstructured meshes. Additionally, some algorithms are difficult to parallelize, and often lead to mass or volume conservation errors over time. In this work, we demonstrate the use of a control volume finite element method (CVFEM) for large-scale parallel simulations of multiphase flows on unstructured meshes. CVFEM combines the flexibility of a finite element interpolation scheme with the robust conservation properties of finite volumes. We convert the advection and redistancing of the level set into a form that can be solved by CVFEM and demonstrate that volume is conserved to a high degree of accuracy for multiphase flow problems. We demonstrate that a diffuse interface description obtained from the level set field allows the straightforward inclusion of complex physical phenomena occurring at the interface between two phases. These interfacial forces, such as surface tension and thermocapillary effects, become significant in engineering applications that exhibit highly localized phenomena including melting and subsequent flow of molten metals in additive manufacturing processes.

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Title: Simulations of Droplet Collision with Cahn-Hilliard Equation on Multi-GPU Cluster

Author(s): Tzu-Chun Huang, Chien-Yi Chang, *Chao-An Lin, *National Tsing Hua University*.

Three-dimensional liquid droplet collision is simulated using Cahn-Hilliard equation on multi-GPU cluster. The capability of the model is first validated by contrasting the predicted frequency of the single droplet oscillation with analytical solution. Coalescence and stretching separation phenomena of two colliding droplets are further studied in terms of two dimensionless variables, Weber number and impact parameter. The predicted results are consistent with benchmark solutions, showing the capability of the model. Further, a MPI based multi-GPU cluster implementation is conducted. Methodology to achieve good scalability is also addressed.

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14th U.S. National Congress on Computational Mechanics
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Title: Inf-sup Stable Computational Methods for Strongly Coupled Porous Media

Author(s): *Christian Linder, Andreas Krischok, Berkin Dortdivanlioglu, *Stanford University*.

The modeling of the interaction between the solid skeleton and an inter-penetrating fluid in porous materials has been a highly active field of research since the early defining works by Biot. In the context of the finite element method it has been recognized early that in highly coupled situations the satisfaction of the well-known inf-sup condition is mandatory for mixed formulations and that the same interpolation schemes that guarantee stability in cases such as Stokes flow or incompressible elasticity provide stable results in poroelasticity as well. A rigorous mathematical proof of certain elements is however unfeasible in many cases and numerical tests have been proposed to judge whether a proposed interpolation scheme is reliable. While this test has been successfully evaluated for standard cases such as Stokes flow, an evaluation for poroelastic problems remains unsatisfactory. This contribution presents ideas how a numerical test can be evaluated successfully in the case of poroelasticity to judge whether a novel interpolation scheme is reliable and hence guaranties uniqueness and necessary stability estimates. Based on these observations we evaluate a number of recent schemes that have recently been proposed in our research group. We present a novel low-order mixed finite element formulation based on an incompatible strain enhancement that provides inf-sup stability while preventing well-known hourglass modes in the limit of large deformations. In addition, in the context of isogeometric analysis we prove the stability of a variety of interpolation schemes based on degree-elevated methods and subdivision-based methods in numerical tests to provide alternatives to classical schemes that, while stable in classical finite element schemes, can fail to provide inf-sup stability. The capability of the proposed schemes is underlined in exemplifying numerical examples including the consolidation of saturated soil under footings and swelling tests of polymeric gels.

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Title: Mesh Generation for Large-Scale Multi-Physics Simulations Using HPC Architectures

Author(s): *Andreas Lintermann, *JARA-HPC, RWTH Aachen*.

The continuous advancement of HPC architectures enables the simulation of multi-physics problems at large-scale with an unexpected precision. Such computations necessitate highly-resolved meshes to simulate the underlying physics with high fidelity. Serial mesh generation is limited by the available memory and the computational costs rendering such an approach unfeasible for large problem sizes. We present an algorithm that automatically constructs octree-based hierarchical Cartesian meshes in parallel on state-of-the-art HPC systems for complex geometries. The meshes feature local refinement, periodicity, allow for optimal simulation load-balancing, and distribute the geometry for memory-efficient computations. Domain decomposition is treated by a mixed Hilbert- and z-curve strategy, i.e., on a coarse refinement level the mesh is parallelized by partitioning along a Hilbert curve and by considering the number of descendants per cell on the according level. Finer levels are stored by depth-first traversal in the octree. The mesh generation scales across hundreds of thousands of computational processes and generates meshes with a number of cells on the order of O(10^11) in a short amount of time. Unlike other approaches, the meshes can be employed for simulations on a quasi-arbitrary number of processes and decomposition is performed on the fly in a pre-processing step. Furthermore, the parallelized geometry enables a reduction of the time spent for geometry pre-processing and the globally allocated memory by a factor in the order of the numer of processes. The mesh generation is integrated into a modular framework to simulate compressible and quasi-incompressible fluid dynamics by means of a finite-volume or a lattice-Boltzmann method. A level-set solver enables the simulation of moving boundaries while a Lagrangian particle solver can be coupled to track individual particles. A discontinuous Galerkin method permits aeroacoustics simulations. The numerical methods to solve for the governing equations of the involved physics operate on the same mesh created by our parallel approach and weighting coefficients per cell can be introduced to balance coupled simulations. Different examples from technical applications as well as from the field of biofluid mechanics are used to validate and corroborate the functionalities of the meshing method.

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Title: Double Well Potentials and Nonlocal Brittle Fracture Modeling

Author(s): *Robert Lipton, *LSU*.

The dynamic fracture of brittle solids is a particularly interesting collective interaction connecting both large and small length scales. Apply enough stress or strain to a sample of brittle material and one eventually snaps bonds at the atomistic scale leading to fracture of the macroscopic specimen. We discuss a nonlocal model [2],[3],[4],[5],[6] of peridynamic type [7] for free crack propagation. The force interaction is derived from a double well strain energy density function, resulting in a non-monotonic material model. The material properties change in response to evolving internal forces eliminating the need for a separate phase field to model the fracture set. The model can be viewed as a regularized fracture model. In the limit of zero nonlocal interaction, the model recovers a sharp interface evolution characterized by the classic Griffith free energy of brittle fracture with elastic deformation satisfying the linear elastic wave equation off the crack set. We illustrate the model with numerical examples [1], [7]. References [1] P. Diehl, R. Lipton, M. A. Schweitzer, Numerical verification of a bond-based softening peridynamic model for small displacements: Deducing material parameters from classical linear theory, Institute for Numerical Simulation University of Bonn Preprint No. 1630 December 2016. [2] P. Jha and R. Lipton, Numerical Analysis of Nonlocal Fracture Models in Holder Space, arXiv:1701.02818v3 [math.NA] 25 Jan 2017. [3] R. Lipton, Dynamic brittle fracture as a small horizon limit of peridynamics, Journal of Elasticity, 117, pp. 21–50 (2014). [4] R. Lipton, Cohesive dynamics and brittle fracture, Journal of Elasticity, 124, Issue 2 (2016), pp. 143-191. [5] R. Lipton, S. Silling, and R. Lehoucq, Complex Fracture Nucleation and Evolution wth Nonlocal Elastodynamics. February 2, 2015, arXiv:1602.00247. [6] R. Lipton and E. Said, Energy balance and damage modeling using dissipation potentials for state based peridynamic fracture evolution. Preprint April 2017. [7] S. A. Silling, Reformulation of elasticity theory for discontinuities and long-range forces, Journal of the Mechanics and Physics of Solids, 48 (2000), pp. 175–209.

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Title: An Agile Computational Approach to Crystal Plasticity

Author(s): *David Littlewood, Coleman Alleman, Guy Bergel, James Foulk, Alejandro Mota, Hojun Lim, *Sandia National Laboratories*.

Crystal plasticity constitutive models are complex and highly nonlinear, requiring innovative numerical strategies and software implementations that are both robust and efficient. A primary challenge is the formation and solution of the nonlinear systems of equations within the state update routine, which often represent a significant fraction of a simulation code's execution time. We present a computational approach for crystal plasticity that utilizes advanced software tools for the inclusion of multiple numerical methods and multiple physics. Primary elements of our approach are the use of automatic differentiation and a nonlinear solver package designed specifically for use within constitutive models. The result is a constitutive model that includes multiple flow rules and hardening laws, and that supports a number of nonlinear, coupled residual formulations for implicit integration of the state variables. We investigate the numerical characteristics of power-law and thermal-activation flow rules within the context of the constitutive model, as well as isotropic linear, slip-based, and dislocation-density-based hardening rules. Also discussed is the impact of various nonlinear solver strategies and the use of different state variables as the unknowns in the nonlinear system, e.g., slip increments and hardness values. Finally, demonstration calculations are presented in which the crystal plasticity model is exercised within both single-scale and multiscale simulations.

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Title: A New Simple Multidomain Fast Multipole BEM

Author(s): *Yijun Liu, Shuo Huang, *University of Cincinnati*.

A simple multidomain fast multipole boundary element method (BEM) for solving potential problems is presented in this talk, which can be applied to solve a true multidomain problem or a large-scale single domain problem using the domain decomposition concept. In this multidomain BEM, the coefficient matrix is formed simply by assembling the coefficient matrices of each subdomain and the interface conditions between subdomains without eliminating any unknown variables on the interfaces. Compared with other conventional multidomain BEM approaches, this new approach is more efficient with the fast multipole method, regardless how the subdomains are connected. Instead of solving the linear system of equations directly, the entire coefficient matrix is partitioned and decomposed using Schur complement in this new approach. Numerical results show that the new multidomain fast multipole BEM uses fewer iterations in most cases with the iterative equation solver and less CPU time than the traditional fast multipole BEM in solving large-scale BEM models. A large-scale fuel cell model with more than 6 million elements was solved successfully on a cluster within 3 hours using the new multidomain fast multipole BEM.
Reference: [1] S. Huang and Y. J. Liu, “A new simple multidomain fast multipole boundary element method,” Computational Mechanics, 58, No. 3, 533–548 (2016).

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Title: A Finite Element Based Method for Simulating Surfactants Spreading on Liquid Films

Author(s): *Yingjie Liu, Christian Peco, John Dolbow, Guglielmo Scovazzi, *Duke University*.

We present a comprehensive framework for simulating the spreading of surfactants on liquid films. Surfactants typically have a lower surface tension compared to the underlying liquid film. When a drop of surfactant is introduced to a liquid film resting on a solid substrate, the variation in the surfactant concentration induces a surface tension gradient which gives rise to a Marangoni force and flow of the underlying fluid. The spreading process strongly depends on the thickness of the underlying liquid film. For thick films, the spreading front Rs scales with time t as Rs ~ t^{3/4}, but as Rs ~ t^{1/4} for thin films. Furthermore, for extremely thin films, the spreading process exhibits fingering instabilities. Although these problems have been studied for over a decade, a robust fully coupled numerical method has yet to be proposed. For thin liquid films, the Navier-Stokes equations can be reduced to a lubrication equation [1]. We propose a fully coupled finite element method which provides higher flexibility and computational efficiency compared to the finite volume and finite difference methods. Simulations using this model satisfy the t^{1/4} law and successfully reproduce the fingering phenomena. We also propose a new model that takes into account the surface roughness and its relationship to the onset of the instabilities. When the underlying liquid film is sufficiently thick, inertial effects cannot be disregarded [2]. In our approach, we employ an asymptotic analysis and propose a high order inertial lubrication model. The fluid velocity is characterized by the bulk Navier-Stokes equations, while the surfactant concentration and the evolution of the free surface are modeled by advection-diffusion equations. We proposed a robust finite element method to approximate the solution to this system, which involves a non-trivial coupling between the PDEs on the bulk and evolving surface. We demonstrate that the method successfully reproduces the t^{3/4} scaling for the spreading of the surfactant. We then investigate the influence of obstacles on the surface and the amount of injected surfactant on the spreading process. Keywords: Lubrication; Navier-Stokes; Fingering; Surfactants References [1] Jensen, O. E. and Grotberg, J. B., 1992. Insoluble surfactant spreading on a thin viscous film: shock evolution and film rupture. Journal of Fluid Mechanics 240, 259–228. [2] Rojas, N.O., Argentina, M., Cerda, E. and Tirapegui, E., 2010. Inertial Lubrication Theory. Physical Review Letters 104, 187801

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Title: Variational Multiscale Method for Incompressible Solid Dynamics with Application to Biological Tissues

Author(s): *Ju Liu, Vijay Vedula, Alison Marsden, *Stanford University*.

Biological tissues are predominantly made of nearly incompressible materials. This material property requires special consideration in the design of numerical methods. Traditional mixed finite element methods require special displacement-pressure elements to satisfy the inf-sup condition. In particular, low-order tetrahedral elements are known to be intractable for incompressible materials. On the other hand, for complex geometries like patient-specific arterial and cardiac walls, automatic meshing is still confined to tetrahedral elements. The variational multiscale method was initially developed in the context of fluid mechanics. With the aid of the VMS, convenient implementations, such as the linear equal-order velocity-pressure element pair, can be applied to solve the incompressible Navier-Stokes equations. Over the years, extension of the VMS to nonlinear solid mechanics has been pursued by several groups [1,2]. In this work, we will first derive a general continuum model that can conveniently recover the incompressible Navier-Stokes equations as well as the finite hyperelasticity. In doing so, the well-established VMS scheme for large eddy simulations in incompressible flows can be naturally extended to the solid mechanics equations. We will spatially discretize the equations using linear tetrahedral elements. We choose the generalized-alpha method for the temporal discretization. Applications to biomechanical problems will be presented to demonstrate the effectiveness of the proposed method. References: [1] S. Rossi, N. Abboud, and G. Scovazzi. Implicit finite incompressible elastodynamics with linear finite elements: A stabilized method in rate form. Computer Methods in Applied Mechanics and Engineering, 311:208–249, 2016. [2] A.J. Gil, C.H. Lee, J. Bonet, M. Aguirre. A stabilised Petrov-Galerkin formulation for linear tetrahedral elements in compressible, nearly incompressible and truly incompressible fast dynamics. Computer Methods in Applied Mechanics and Engineering, 276:659–690, 2014

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Title: A Lattice-Boltzmann Based Multiscale Approach for Simulating Nanoparticle Transport in Cellular Blood Flow

Author(s): *Zixiang Liu, Yuanzheng Zhu, Cyrus Aidun, *Georgia Institute of Technology*; Rekha Rao, Jonathan Clausen, *Sandia National Laboratories*.

The bio-transport of the intravascular nanoparticle (NP) is influenced by both the complex cellular flow environment and the NP characteristics. To be able to computationally simulate such complex transport phenomenon is of far-reaching significance to the development of the NP therapeutics, and yet challenging due to the large discrepancy of the scales between the NP and the cellular components, e.g., the red blood cell (RBC). Recently, a lattice-Boltzmann (LB) based multiscale simulation method has been developed to capture both the NP-level and cellular level transport phenomenon at high computational efficiency. The basic components of this method include the LB treatment for the fluid phase, a generalized worm-like-chain (WLC) network model for RBCs and deformable boundaries, and a Langevin dynamics (LD) approach to capturing the motion of the solute NPs. Two-way coupling schemes are established to ensure comprehensive interactions between each component. This approach is extensively validated through benchmark cases (such as the relaxation of a single particle with initial momentum, single particle self-diffusion, and dispersion of concentrated particles, etc.) with good agreements with the analytical counterparts. The verified method is then applied to study the migration of NPs in a cellular capillary vessel. It is found that the Brownian diffusion, compared to the shear-induced diffusion, is the predominant driver for the margination of NPs (1~100 nm). A scaling factor is also introduced to quantify the NP diffusion process. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: B-Spline Based Topology Optimization for Metal Hybrid Additive-Subtractive Manufacturing

Author(s): *Jikai Liu, Albert To, *University of Pittsburgh*.

Hybrid additive-subtractive manufacturing is an emerging technology, which is capable of fabricating complex raw part through additive manufacturing (AM) and then finishing the part to meet surface and dimensional requirements through subtractive machining. Therefore, a large design space could be explored to ensure design creativity, and the derived size, form, and surface quality satisfy engineering requirements. However, there are key current issues that are impeding the marriage between hybrid manufacturing and topology optimization: 1) Inability to connect the topology optimization result to commercial CAD/CAM system for post-editing and manufacturing simulations, and 2) Difficulty in post-machining topology optimized AM parts due to their highly complex shapes. To fix these issues, this research contributes a B-spline based topology optimization method capable of interfacing commercial CAD/CAM systems and accounting for post-machining requirements. Specifically, both the B-spline control points and feature modeling history will be adopted as the shape and topology variables, where the 'feature modeling history' topological derivative concept is novel and highlighted. Both the B-spline information and feature modeling history are important assets to interface CAD for user-friendly post-editing; and the topology optimized AM component would be composed of both freeform surfaces and machining-friendly surfaces, which fits the scope of hybrid additive-subtractive manufacturing. The technology developed will significantly shorten the design phase during new AM product development, which will potentially lead to wider adoption of AM. Effectiveness of the proposed method will be proved through studies of several real parts.

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Title: Per-Residue Energetic Analysis Clarifies the Mechanism of the Binding Strength inside Microtubules

Author(s): *Ning Liu, Ramana Pidaparti, Xianqiao Wang, *University of Georgia*.

Microtubules (MTs), the essential structural element of cells, are long filamentous hollow cylinders whose surfaces form lattice structures of $\alpha\beta$-tubulin heterodimers. In order to better capture and understand the self-assembly of MTs from single α and β tubulins, it is vital for us to calibrate the energetic interactions between any pair of α and β tubulins with atomic resolutions. These interactions play a critical role in determining the mechanical properties and structural stability of the MTs. Thus, we carry out a variety of full atomistic simulations to investigate the interaction properties, such as adhesion energy, tensile strength, and shear strength between pairs of α and β tubulins. Results indicate that as the loading velocity decreases, both intra-dimer and inter-dimer stiffness decreases intensively and then stabilizes at an equilibrium value. Moreover, the per-residue energy map shows that the more contact pairs the residue has with the other tubulin, the more contributions it makes to the intra-dimer and inter-dimer binding strength. In addition to its dependence on interaction distance, results also show that the residues with charges, namely arginine (ARG), lysine (LYS), glutamic acid (GLU), aspartic acid (ASP) in one tubulin, tend to have stronger binding interactions with the counterpart tubulin than other residues. Furthermore, the binding strength can be tuned through residue mutation in close contact with the adjacent tubulin. Overall, our results can provide a thorough atomistic understanding of the binding strength inside MTs and help pave the way for the control of self-assembly of $\alpha\beta$-tubulin heterodimers.

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Title: Design Optimization Method for Additive Manufacturing Primary Mirror of Large-Aperture Space Telescope

Author(s): *Shuitan Liu, Rui Hu, *Dalian University of Tech.*.

The principal way to reduce the mirror weight is to use a honeycomb structure on the mirror back with the premise of meeting the surface shape requirements of the mirror face. However, for the existing commonly used mirror fabrication method, it is difficult to manufacture the sandwich mirror structure with closed-back honeycomb holes. Accordingly, the lightweight holes on the mirror back are generally open or half-open form. Additive manufacturing (AM) technologies can realize the fabrication of a complex internal structure that makes the closed-back sandwich mirror manufacturable and an alternative to achieve a higher performance. In this paper, a novel topology optimization model for closed-back primary mirror of a large-aperture space telescope is proposed. First extrusion constraints are considered in the optimization model to get the layout design of stiffeners. Furthermore, a simply-connected constraint, as one type of constraints in AM is considered to avoid enclosed voids in the structures, in this way, the unsintered powders can be removed from the side through connected paths. Through solving the proposed model, a new closed-back sandwich mirror configuration, whose internal core is composed of non-closed tree-like vertical stiffening webs, is achieved. In addition, the thicknesses of the internal stiffening webs are optimized for minimizing the total mass with the constraint of surface shape error of the mirror face. Compared with the classical half-open triangular honeycomb sandwich mirror, the RMS (root mean square) of the surface shape error for the 2 meters aperture mirror under gravity parallel to the optical axis presented in the design example is reduced 34.3% with the same weight; Compared with the open-back double-directional multi-arch mirror, the optical performance of mirror surface under gravity is somewhat better, meanwhile, the total weight is reduced by 21.1%. The optimization design results illustrated the effectiveness of the presented method. Keywords: space mirror; lightweight design; topology optimization; additive manufacturing; simply-connected constraint References 1. Y. Li and H. Yang, “Large aperture lightweight primary mirror design method using topology optimization,” Opt. Technique 34, 236-238 (2008). 2. S. Liu, Q. Li, W. Chen, L. Tong and G. Cheng, "An identification method for enclosed voids restriction in manufacturability design for additive manufacturing structures," Frontiers of Mechanical Engineering 10, 126-137 (2015).

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Title: Reduced Order Modeling of Knitted Textiles Geometry and Deformation

Author(s): *Dani Liu, Daniel Christe, Bahareh Shakibajahromi, Chelsea Knittel, David Breen, Genevieve Dion, Antonios Kontsos, *Drexel University*.

Knitted textiles are hierarchically structured materials. Compared to other materials such as fiber-reinforced composites or metals, knitting provides much finer control over the manufacturing process and creates a variety of multi-scale structures using a range of input materials. Mechanical behavior of knitted textiles is difficult to be efficiently predicted by traditional computational methods due to its complicated, entangled internal structures. Flexural motion, interaction activities and hierarchical structure of or between subcomponents contribute to a complex behavior with high nonlinearity and instability of knitted textiles. This talk is focused on developing a Reduced Order Model (ROM) for knitted textiles based on the actual behavior obtained by 3D/full models used in Finite Element (FE) simulations. In order to construct such ROM from direct models of the actual knitted geometry as this is dictated by the topology imposed by stitch level operations, yarn to yarn interaction activities, including compression, slide and rotation are firstly investigated by implementing different interaction definitions. The interfacial forces and relative motions between yarn surfaces are shown to play a significant role in the global material response, which also help to condense the geometrical/behavior information of 3D full model into two elements: the spatial curvature of the loop and the contact zones between yarns. Based on this information, a 3D ROM constructed by using the center lines of the yarn loop and connectors that link the initial contact points in the 3D full model is presented. Discretized by linear beam elements (center lines) and equipped with kinematic constraints or spring-like connectors, the ROM is demonstrated to be a good approximation of the 3D full model for a range of boundary conditions.

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Title: Multi-Physics Modeling of Multiple-Track Defect Mechanisms in EBSM

Author(s): *Wing Kam Liu, *Northwestern University*.

Metallic powder bed-based additive manufacturing technologies have many promising attributes. The single track acts as one fundamental building unit, which largely influences the final product quality, such as the surface roughness and dimensional accuracy. A high-fidelity powder-scale model based on the Finite Volume Method is developed to predict the detailed formation processes of single track defects, including the balling effect and single track nonuniformity. These processes are difficult to observe in experiments, and previous studies have proposed different or even conflicting explanations. Our study clarifies the underlying formation mechanisms, reveals the influence of key factors, and guides the improvement of fabrication quality. Additionally, the manufacturing processes of multiple tracks along S/Z-shaped scan path are simulated to further understand the defects in complex structures.

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14th U.S. National Congress on Computational Mechanics
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Title: High-Order Incompressible Computational Fluid Dynamics on GPUs and Co-Processors

Author(s): *Niki Loppi, Peter Vincent, *Imperial College London*; Freddie Witherden, Antony Jameson, *Stanford University*.

GPU and co-processor accelerated Computational Fluid Dynamics (CFD) has become increasingly popular over the past decade. Modern hardware architectures are characterised by an excess of compute capability relative to memory bandwidth. This makes them well suited to solving temporally explicit and spatially compact discretisations of hyperbolic conservation laws. However, classical pressure projection based Incompressible Navier-Stokes formulations do not fall into this category. Hence GPU/co-processor accelerated incompressible CFD still remains relatively unexplored as a topic area. One attractive formulation for solving incompressible problems on GPUs/co-processors is the method of artificial compressibility. When used together with explicit dual time stepping and a high-order Flux Reconstruction discretisation, the majority of operations can be cast as compute bound matrix-matrix multiplications that are well-suited for GPUs/co-processors. Building on the approach of Cox et al. [1], a 3D incompressible solver based on artificial compressibility with dual time stepping was implemented in the open-source high-order accurate PyFR framework, which can target a range of modern platforms. The implementation will be described in detail, and a range of convergence acceleration techniques for the inner pseudo-iterations will be investigated, including a polynomial multigrid, explicit maximum stability schemes and local time time stepping. A 3D jet simulation at Reynolds number 10,000 will also be presented. [1] C. Cox, C. Liang, and M.W. Plesniak. A high-order method for solving unsteady incompressible Navier-Stokes equations with implicit time stepping on unstructured grids. AIAA Scitech Aerospace Sciences Meeting, 2015. [2] F.D. Witherden, A.M. Farrington, and P.E. Vincent. PyFR: An open source framework for solving advection–diffusion type problems on streaming architectures using the flux reconstruction approach. Computer Physics Communications, 185: 3028–3040, 2014.

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Title: A Computational Framework for Tissue-Scale, Patient-Specific Prediction of Prostate Cancer Growth

Author(s): *Guillermo Lorenzo, *Universidade da Coruña*; Michael Scott, *Brigham Young University*; Kevin Tew, *Coreform*; Thomas Hughes, *The University of Texas at Austin*; Hector Gomez, *Purdue University*.

Predictive Medicine is a novel trend in Medicine whose aim is to forecast clinical outcomes of diseases and design optimal treatments on a patient-specific basis. This new approach features methods based on mathematical modeling and computer simulations. Predictive Medicine complements the statistical and experiential basis of diagnosis and treatment planning, which characterize current medical practice. Prostate cancer (PCa) is a major type of cancer among men worldwide and an ideal candidate to benefit from Predictive Medicine for three main reasons: first, the prostate is small enough to pursue tissue-scale simulation; second, clinical protocols for PCa include medical imaging techniques that provide the patient's organ and tumor geometries, and third, tumor growth can also be estimated by measuring serum prostate-specific antigen (PSA, a PCa biomarker in blood). The history of medical images and PSA tests may enable in vivo validation of the modeling and simulation technologies. We present a continuous model for organ-confined PCa growth. We use the phase-field method to account for the healthy-to-tumoral transition and diffusion-reaction equations to model the dynamics of nutrients and the production of PSA. The growing tumor produces a mass effect that induces the deformation of the prostate. The stress fields may exert an inhibitory effect on the development of the tumor. Hence, we also explore the mechanical coupling of this deformation with tumor dynamics. Our simulations leverage Isogeometric Analysis (IGA) using a hierarchical basis of NURBS to accurately and efficiently compute tumor growth. This model can reproduce the growth patterns of PCa. Indeed, it captures a known shape instability from spheroidal to fingered morphology. Our simulations suggest that this change in shape enables the tumor to escape starvation, hence contributing to cancer survival and further development. We also used our model to perform tissue-scale, patient-specific simulations of PCa cases, based on the patient's prostatic anatomy extracted from medical images. These simulations show tumor progression similar to that seen in clinical practice. We analyze the implications of tumor morphology in the diagnosis and prognosis of the disease both considering and neglecting the deformation induced by the growing tumor. References: [1] G. Lorenzo, M.A. Scott, K. Tew, T.J.R. Hughes, Y.J. Zhang, L. Liu, G. Vilanova, and H. Gomez, "Tissue-scale, personalized modeling and simulation of prostate cancer growth", Proc. Natl. Acad. Sci. U.S.A., 113 (48), E7663-E7671 (2016). [2] M.A. Scott, D.C. Thomas, and E.J. Evans, "Isogeometric spline forests", Comput. Methods Appl. Mech. Engrg., 269, 222-264 (2014).

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Title: Efficient High-Order Time-Stepping Methods for 3D Incompressible Flows

Author(s): *Kak Choon Loy, Yves Bourgault, *University of Ottawa*.

The numerical solution of the incompressible Navier-Stokes equations typically gives rise to saddle point problems which are numerically challenging to deal with, especially when computing three-dimensional flows. We present strategies to tackle the challenges while solving the three-dimensional Navier-Stokes equations using mixed finite element methods. We use Taylor-Hood (P2-P1) elements since they are known to be very accurate. For 3D computations, the resulting linear system leads to large saddle point problems where velocity components are tightly coupled to pressure. This linear system is indefinite and poorly conditioned, which produces slow convergence of iterative solvers. A robust preconditioner is usually required but not easy to devise and expensive to compute. Inspired by the work of Guermond and Minev (2015), we present a high-order time-stepping method which transforms this saddle point problem into subproblems with symmetric and positive definite matrices. The idea is based on deferred correction and provides an alternative velocity-pressure splitting. A semi-implicit approach is used for the extrapolation of the nonlinear term, which allows the global matrices and the implemented preconditioner (the Hierarchical Iterative Parallel Solver - HIPS), all to be built only once. Our talk will also address the potential of the grad-div splitting from (Guermond & Minev, 2016) to reduce further the computational burden of computing 3D flows with the Taylor-Hood element. We showcase several test cases using manufactured solution, 3D steady (Re=100 - 1 000) and unsteady (Re=1 970) lid-driven cubic cavity, and 3D unsteady flows around the circular cylinder (Re=100) and sphere (Re=300). The proposed strategies will be shown to be efficient and accurate for computing 3D incompressible flows. References: Guermond JL and Minev PD. 2015. High-order time stepping for the incompressible Navier–Stokes equations. SIAM Journal of Scientific Computing, 37: 6, pp. A2656–A2681. Guermond JL and Minev PD. 2016. High-order time stepping for the Navier–Stokes equations with minimal computational complexity. Journal of Computational and Applied Mathematics, 310, pp. 92- 103.

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Title: Computational Homogenization of the Nonlinear Electrical Behavior of Graphene/Polymer Nanocomposites

Author(s): *Xiaoxin Lu, Jinbo Bai, *Ecole Centrale Paris*; Julien Yvonnet, Fabrice Detrez, *East Paris university*.

Tunnelling effect is a possible mechanism to explain the apparent large electric conductivity and nonlinear electric behavior of graphene-reinforced nanocomposites with polymer matrix. In this work, a numerical modeling framework is proposed to evaluate the effective electric conductivity in polymer composites reinforced with graphene sheets, taking into account the electrical tunnelling effect, which allows conduction between graphene sheets at nanometric distances. We introduce a nonlinear Finite Element formulation and a numerical methodology to model the nonlocal and nonlinear effects introduced by the tunnelling effect conduction model within the polymer matrix between close graphene sheets. In addition, to avoid meshing the thickness of the graphene sheets and in view of their very high aspect ratio, a highly conducting surface model is employed. The computed effective conductivity is evaluated over representative volume elements containing arbitrary distributed graphene sheets. The results exhibit tendencies and percolation thresholds which are in qualitative agreement with the available experimental results.

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Title: A Space-Time 'Computational Vademecum' Based Approach for Multi-Parametric Simulations of Welding Processes

Author(s): *Ye Lu, Nawfal Blal, Anthony Gravouil, *Univ Lyon, INSA-Lyon, CNRS UMR*.

In spite of the impressive progresses in computer science, traditional approaches reach some limitations when dealing with nonlinear parametric problems, like in inverse identification or optimization of the welding or additive manufacturing processes. A very large number of solutions of the concerned model has to be computed for different values in the problem parameter space. Moreover, real-time simulations are usually needed for rapid identification or optimization processes. This remains intractable with traditional computational approaches due to the increasing degrees of freedom and complexity of the models. In order to deal with parameter space of high dimensions, keeping lower cost of computational time and memory storage, use can be made of reduction order model approaches (e.g. [1]). In this study, a novel non-intrusive strategy for construction of multiparametric computational vademecum, dedicated to parametric studies of welding, is presented. This is based on a set of offline precomputed standard finite element solutions, which is selected in an appropriate way in the concerned parameter space. The Higher-Order Proper Generalized Decomposition method (HOPGD) [2] is then used for searching a separated representation of variables (space, time and mastering variables). A residual-based accelerator [3] is successfully integrated in order to accelerate the reduced basis construction. Once the separated parameter functions are constructed, new solutions for new parameter values can be rapidly obtained by interpolation. In order to control the accuracy of solutions with reasonable cost, a multigrid-based refinement method is proposed to sample the parameter space. These parametric solutions form hence a computational vademecum that leads to real time space-time responses for any input parameter value. It can be therefore used by engineers to make real time decisions for welding processes optimization. [1] S. Niroomandi, I. Alfaro, E. Cueto, F. Chinesta, Real-time deformable models of non-linear tissues by model reduction techniques Comput. Methods Progr. Biomed., 91 (2008), pp. 223–231. [2] D. Modesto, S. Zlotnik, A. Huerta, Proper generalized decomposition for parameterized helmholtz problems in heterogeneous and unbounded domains: Application to harbor agitation, Computer Methods in Applied Mechanics and Engineering 127–149, 295 (2015). [3] I. Ramière, T. Helfer, (2015). Iterative residual-based vector methods to accelerate fixed point iterations. Computers & Mathematics with Applications, 70(9), 2210-2226.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Simulation of Additive Manufacturing and Techniques to Reduce the Computational Time

Author(s): *Andreas Lundbäck, Andreas Malmelöv, Johan Lindwall, Lars-erik Lindgren, *Luleå University of Technology*.

Additive manufacturing (AM) is a manufacturing method that is becoming increasingly popular by the day. One of the reasons is the ability to produce complex structural components of near net shape. Adding features to existing structures is also a possibility. The method can even be used to repair existing components. A lot of work that is carried out with AM is based on trial and error. Finding process parameters such as heat input, scan speed and scan strategy is mainly carried out by physical experimentation. Depending on the current material and the application of the final component, this approach can be time consuming and costly. With the aid of simulations, it may be possible to reduce the number of experimental iterations and at the same time increase the knowledge about the process such as the size of the process window. The thermal history dictates the microstructure evolution and when building components in metallic glass the cooling ratio is of outmost importance. However, if deformations and residual stresses is of interest then a coupled thermo-mechanical model is in most cases necessary. Particularly the powder bed method poses some great challenges to simulation. For building a small component still several thousands of layers are required. This renders in very long simulation times if even possible to simulate. In the following presentation, examples of methods that has been investigated in order to reduce the computational time will be presented. One of the methods are lumping of added layers. This means that several passes or layers has been merged and is treated as one. In the current example, blown powder and a laser heat source, the computational time was reduced down to 5% compared to a fully detailed analysis with maintained accuracy of the resulting deformations. Another method is dynamic local mesh adaptivity. In this case a cylinder is built with the powder bed method. Each layer is 70 μm thick and the height of the cylinder is 80 mm. This means that more than thousand layers is added. By refining the mesh only at the active layer and some layers below it is possible to resolve the process. When the thermal gradient has declined the elements are coarsened in order to keep the problem at a manageable size with reasonable computational times. The methods described above introduces simplifications that may or may not be acceptable. It depends on the scope of the simulation and what result that is sought for.

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July 17-20, 2017, Montreal, Quebec, Canada

Title: Numerical Simulation of Temperature Fields in Powder Bed Fusion Process by Using Hybrid Point and Line Heat Source Model

Author(s): *Zhibo Luo, Yaoyao Zhao, *McGill University*.

Powder bed fusion (PBF) process is one of the seven Additive Manufacturing processes. It is capable of producing complex geometrical part with less material and energy consumption compared with conventional manufacturing methods. The performance of PBF processed part is mainly controlled by many process parameters such as scanning speed, scanning pattern, scanning strategy, layer thickness, etc. Usually these parameters are optimized through detailed experiments which are time-consuming and costly. Therefore, many researchers utilize numerical methods to investigate the effects of these process parameters on temperature fields and thermal stress fields. As the laser/electron beam introduces huge temperature gradients within the irradiated region, which will result in the distortion even delamination of solidified layers. Therefore, the study of history of temperature distribution is the basic and crucial step in the modeling of PBF process. The finite element method is the most commonly used numerical method for predicting temperature and stress fields in PBF process. Most of the current research utilizes moving Gaussian point heat source as heat input to model the temperature distribution of a part. However, due to the small diameter of laser/electron beam, a small enough time step is required to accurately model the real heat input, which will lead to a significant computational burden. In this research, a hybrid point and line heat source model is developed, which makes the modeling of PBF process efficient without losing too much accuracy. In addition, an adaptive mesh scheme, which is capable of dynamically refining the mesh near the beam spot and coarsening the mesh far away from the beam spot, is adopted to accelerate the simulation process. Specifically, Gaussian moving point heat source is applied to the region of interest where accuracy is more concerned such as the temperature field within overhang feature. While line heat source is applied to the region of interest where efficiency is more concerned such as temperature field within the inner region of a square. For the line heat input, the entire scanning track is broken up into several segments. Each segment is irradiated for several relatively large time increments. The simulation result shows that the temperature fields by using hybrid line and point heat source model are comparable to the temperature fields by using moving Gaussian point heat source model, and much less central processing unit time is required when the hybrid heat source is applied.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A New Predictor-Corrector Method for Efficient Modeling of Surface Effects

Author(s): *Mitchell Luskin, Andrew Binder, *University of Minnesota*; Christoph Ortner, *University of Warwick*.

The regular Cauchy-Born method is a useful and efficient tool for analyzing bulk properties of materials in the absence of defects. However, the method normally fails to capture surface effects, which are essential to determining material properties at small length scales. Here, we present a corrector method that improves upon the prediction for material behavior from the Cauchy-Born method over a small boundary layer at the surface of a material by capturing the missed surface effects. We justify the separation of the problem into a bulk response and a localized surface correction by establishing an error estimate, which vanishes in the long wavelength limit.

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14th U.S. National Congress on Computational Mechanics
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Title: Diffusion of Band-3 Protein and Vesiculation in the Healthy and Defective Red Blood Cell Membrane

Author(s): He Li, *Brown University*; Yihao Zhang, Vi Ha, *George Lykotrafitis, *University of Connecticut*.

In this work, a two-component red blood cell (RBC) membrane model was developed to measure the band-3 protein diffusion and vesiculation in the normal RBC and RBC with defective membrane proteins found in hereditary elliptocytosis (HE) and hereditary spherocytosis (HS). First, we quantified the relation between the band-3 diffusion coefficients and the percentage of protein defects in HE and HS RBCs. We concluded that in the HE RBCs, band-3 diffusion is featured as anomalous and confined diffusion at low spectrin network connectivity and high spectrin network connectivity, respectively. However, in the case of HS RBCs, band-3 diffusion can be approximately described as confined diffusion at all attraction levels. By comparing the diffusion coefficients measured in HE RBCs and in HS RBCs, we conclude that band-3 mobility is primarily controlled by the connectivity of the membrane skeleton. Finally, we used this model to study how the membrane spontaneous curvature and lateral compression control RBC vesiculation. The results showed that a large spontaneous curvature of the membrane facilitates the formation of small homogeneous vesicles with a diameter less than 40nm. Lateral compression on the membrane generates vesicles with a size comparable to cytoskeleton corral. In HS RBCs, larger-size vesicles, which do not contain cytoskeletal filaments, are released under the same compression ratio as in normal RBCs. Due to the fragmentation of the membrane skeleton, vesicles shed from HE RBCs contain cytoskeletal filaments.

14th U.S. National Congress on Computational Mechanics
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Title: Simulation of Void, Dislocation, and Interphase Defects via A Multiscale Crystal Defect Dynamics Method

Author(s): *Dandan Lyu, *UC-Berkeley*; Shaofan Li, *University of California, Berkeley*.

Crystal defects play an important role in determining material properties at macroscale. For example, dislocations are the origin of plasticity; voids can pin down dislocations, and thus play a vital role in work-hardening. In the present study, a multiscale crystal defect dynamics (MCDD) model is developed to simulate void nucleation, dislocation motion, slip plane formation, and their interactions. The main novelties of present work are: (1) The discrete differential geometry theory is used to construct a scalable non-Bravais lattice model for the coarse-grained defect microstructure, which can model all possible defects inside a crystal; (2) A higher order Cauchy-Born rule (up to the fourth order) is adopted to construct atomistic-informed constitutive relations for various defect process zones, and (3) A hierarchical strain gradient theory based continuum finite element formulation is developed to support a hierarchical multiscale cohesive (process) zone model for various defects simultaneously. The MCDD model is validated by comparisons with the numerical results of molecular dynamics (MD) for three-dimensional nanoindentation of single crystal copper. The efficiency of MCDD method allows us to simulate dynamic evolution of defects at large scales while taking into account atomistic interactions. Numerical simulations have shown that MCDD model can predict dislocation nucleation induced elastic instability automatically, and it may provide a possible solution to study the mechanism of crystal plasticity.

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14th U.S. National Congress on Computational Mechanics
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Title: On the Construction and Use of High-Order Boundary Element

Author(s): *Hang Ma, *Shanghai University, China*; Donghong He, *Shanghai Institute of Applied Mathematics and Mechanics*.

In the boundary element method, compared with the ordinary low-order boundary elements such as the constant, the linear and the quadratic elements, the high-order boundary elements can find their use in the simulation of composite materials [1] containing particles and cracks. The shape function for high-order elements can be constructed readily by Lagrange polynomials. Before an element with fixed order can be used for a given node distribution, however, each shape function has to be specified one by one before programing, resulting in much human cost. In the present work, by rearranging the Lagrange polynomials into the sum of monomials with reduced-order series then by rewriting them in the form of nested products, the coefficient matrix for the shape function of high-order elements can be generated automatically by computer program, leading to the lowest computation cost. The closed surfaces and cracks are simulated by the high-order elements. It is found that the unequally spaced nodes can improve the interpolation accuracy when discretizing the circle or sphere with a single high-order element. Compared with the quadratic elements, the use of high-order element can achieve higher accuracy at the same cost or achieve higher efficiency with less computation cost. [1]Gao XW, Yuan ZC, Peng HF, Cui M, Yang K. Isoparametric closure elements in boundary element method. Computers and Structures 2016,168:1-15 Acknowledgement: The work was supported by the National Natural Science Foundation of China (No.11672173,11272195)

14th U.S. National Congress on Computational Mechanics
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Title: A Multiscale Model for the Oxygen Reduction and Oxidation Reactions in LSCF Based Solid Oxide Cell

Author(s): *Linjian Ma, N.r. Aluru, *Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign*.

Lanthanum Strontium Cobalt Ferrite, La_(1-x)Sr_(x)Co_(1-y)Fe_(y)O_(3-δ)(LSCF), is a mixed ionic-electronic conductor which is widely used in solid oxide cells. However, reaction mechanisms in LSCF based electrodes are not fully understood. Here, we develop a multiscale model combining quantum calculations, transition state theory and continuum modeling for the oxygen reduction and oxidation reactions in LSCF based solid oxide fuel and electrolysis cells, respectively. Quantum calculations are used to obtain the energy barriers for different reaction steps. Transition state theory is used to predict the reaction rate constants for each step based on the energy barriers and vibrational frequencies from quantum calculations. Continuum modeling utilizes the reaction rate constants and predicts the overpotential-current relations. The proposed model yields good quantitative agreement with the overpotential-current data from experiments. The results indicate that oxygen exchange through the LSCF surface, rather than oxygen exchange at the three phase boundary, is the main reactive pathway for a single phase LSCF electrode. The results also highlight that the reaction rate constants on the LSCF surface vary with the oxygen vacancy concentration, which results from the oxygen 2p band shift.

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Title: Inverse Method for Determination of Hardening Parameters of Ductile Materials by a Hardness Test: Numerical and Experimental Aspects

Author(s): *Lucas Q. Machado, Lucival Malcher, *University of Brasilia*.

There are many challenging problems involving the behavior of materials and many techniques have been developed to quantify their properties, defined by different constitutive models. Indentation test is most used to determine hardness of materials but it was noticed that it can be also used to fully characterize elastic-plastic properties from its reaction curve, as it is done with the traditional tensile test. Since it helps making the parametric identification process easier, cheaper and faster, researches have been made to quantify materials parameters from the indentation test. Thus, this work consists in the determination of the hardening curve of ductile materials through a parametric identification process, using an indentation test. A methodology was developed to determine the chosen set of material parameters that describes the hardening curve, using numerical methods that encompasses the golden ratio search, least square method and finite elements. First, a traditional tensile test is performed and the hardening parameters are extracted from it through an inverse parameter identification methodology. In the sequence, a Brinell hardness test is performed and then modeled for simulation in a finite element environment. The same parametric identification routine used for the tensile test is then used for the indentation test and the hardening parameters now are extracted from it. The proposed method numerically replicates the same indentation mark left in the specimen by the indenter. Finally, the hardening curves obtained from traditional and indentation methods are compared to certify the new methodology.

14th U.S. National Congress on Computational Mechanics
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Title: Multiscale Modeling Technique for Non-Linear Composite Materials

Author(s): *Michael Macri, Andrew Littlefield, *ARDEC*.

The defense industry is increasingly incorporating composite materials into military systems, many of which undergo rapid and severe changes in temperature, as well as subject the composites to physical trauma or environmental conditions that can cause micro damage leading to variations of the mechanical properties. For these applications, it is crucial to develop models that can accurately simulate the response of these materials. Composites, in general, are composed of materials that have temperature dependent properties. This dependence leads to nonlinear material simulations, requiring continual updates to the microstructure's response to account for the property changes. Though empirical data can be used to approximate the material properties for an ideal specimens, performing experimentation on composites with nonlinear responses and extracting effective material properties can be extremely difficult. One approach to extract material properties from a composite material without having to perform experimental testing is a numerical approximation method, called the homogenization method. A limitation with the homogenization method is that it suffers from a basic assumption that there is uniformity of the macroscopic fields within each representative volume element (RVE). Hence, this method breaks down in critical regions of high stress gradients. To address this issue, a structural based enrichment method, based on the principles of partition of unity is presented. The principles of partition of unity allows enrichment of the approximation space in localized sub domains using specialized functions that may be generated based on a priori information regarding asymptotic expansions of local stress fields and microstructure. For this presentation, we will focus on incorporating nonlinear effects into the simulation. The research presented reviews the derivation of the enrichment functions needed to represent the micro-structure, which is a piece-wise numerical representation of the micro-displacement to macro-strain relationship. Because of the piece-wise nature of the function, it is dependent on the geometry of the micro-structure, enabling it to contain various micro-structures and material properties.

14th U.S. National Congress on Computational Mechanics
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Title: Peridynamics for Solving Nonlinear Partial Differential Equations

Author(s): *Erdogan Madenci, Mehmet Dorduncu, *University of Arizona*.

Boundary and initial value problems for differential equations arise in almost every branch of science. When suitable, the solutions to these equations with standard finite difference techniques are commonly obtained by reducing the order of differential equation to a sequence of lower order differential equations. If not suitable, their solution requires special techniques such as iterative methods or multi-scale solutions. Such techniques require the approximation of the derivatives at discrete points in the domain. Their solution becomes challenging due to the presence of higher order derivatives, steep variation (discontinuities or sharp gradients) in behavior, nonlinearity and multi-scale solution. This study applies peridynamics for the solution of nonlinear partial differential equations subjected to boundary and initial conditions. The fidelity of this approach is established by considering differential equations that exhibit steep variation (discontinuities or sharp gradients) in behavior, nonlinearity and multi-scale solutions.

14th U.S. National Congress on Computational Mechanics
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Title: A Statistical Surrogate Based Bayesian Approach to Uncertainty Quantification in Brain Injury Criteria

Author(s): *Sandeep Madireddy, *Argonne National Laboratory*; Kumar Vemaganti, *University of Cincinnati*.

Traumatic brain injuries (TBI) lead to approximately 50,000 fatalities annually in the US alone. Finite element (FE) computational models of the head and brain are extensively used to study the effects of impact loading and develop protective gear. In order to use computational models to predict high consequence events like traumatic brain injury, a high level of fidelity is desirable. This is achieved by quantifying in uncertainty in the inputs to the computational model like the material properties, boundary conditions etc. on quantities of interest like the brain injury criteria that indicate the onset of injury. For soft tissues, the material properties are the dominating source of uncertainty. Therefore our goal is to quantify this uncertainty in the material parameters and propagate it to the calculation of the brain injury criterion. We adopt a Bayesian approach to quantifying the uncertainty in the material parameters and a non-intrusive uncertainty propagation approach to obtain the uncertainties in the brain injury criterion. However, as the FE model is computationally expensive, non-intrusive propagation, which involves the execution of the FE model for thousands of samples in the material model parameter space, is not feasible. For this reason, we resort to a Bayesian Gaussian process surrogate model for the injury criterion as a function of the material model parameters using a few hundred FE simulations. A stochastic nonlinear visco-hyperelastic constitutive model is developed to represent the soft tissue in the brain [1,2] and the loading, boundary conditions correspond to impact loading experienced by head in a vehicle crash. The parameters in the constitutive model and those in the surrogate model are estimated using the nested sampling based algorithm MULTINEST [3]. The posterior predictive distribution of the surrogate is then used to propagate the uncertainty in the material parameters to the injury criterion. This enables us to calculate the probability that an injury tolerance is reached for a given impact loading. For the given loading scenario, the probability that mild traumatic brain injury occurs is 85% assuming the maximum principal strain-based injury tolerance for mild TBI is 0.33. [1] S. Madireddy et.al., “A Bayesian approach to selecting hyperelastic constitutive models of soft tissue”, Computer Methods in Applied Mechanics and Engineering, 291 (2015) 102-122. [2] S. Madireddy et.al., “Bayesian calibration of hyperelastic constitutive models of soft tissue”, Journal of the Mechanical Behavior of Biomedical Materials, 59 (2016) 108-127. [3] Feroz F et.al., “Multinest: an efficient and robust Bayesian inference tool for cosmology and particle physics”. Monthly Notices of the Royal Astronomical Society, 398(4):1601–1614, 2009.

14th U.S. National Congress on Computational Mechanics
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Title: Spectral Hybrid Localized Orthogonal Decomposition Method

Author(s): *Alexandre Madureira, *LNCC*; Marcus Sarkis, *WPI*.

We consider a primal hybrid finite element method for elliptic equations with heterogeneous coefficients. It is based on a special space decompositions, as in FETI and TFETI methods, and most of the computations can be done in parallel. The global problems are not affect by the coefficients, and the multiscale coefficients show up in local problems. One of the problems is non-local, but has exponentially decaying solutions, allowing a truncation. We derive an error estimate that requires minimum regularity, and does not depend on restrictions as periodicity, etc, but depends on the contrast of the coefficients. We comment on how to extend the method to account for the high-contrast case as well, based on local spectral problems.

14th U.S. National Congress on Computational Mechanics
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Title: A Constrained Resampling Strategy for Eliminating Short Edges in Voronoi Meshes

Author(s): Mohamed Ebeida, *Sandia National Laboratories*; *Ahmed Mahmoud, Ahmad Rushdi, John Owens, *University of California, Davis*; Ahmed Abdelkader, *University of Maryland*.

In this talk, we introduce a new strategy for improving the quality of a mesh by interpreting quality objectives as geometric constraints for resampling. We focus on the application of our method to process Voronoi meshes with undesired short edges, successfully eliminating them. Furthermore, we also demonstrate how to simplify Delaunay meshes while preserving element quality and eliminate all obtuse angles in a complex mesh. We derive the geometric realization of various objectives using a collection of geometric primitives and describe a toolbox of local resampling operators to improve or preserve quality. Our strategy judiciously combines smoothing and transformation techniques which have previously been used separately in different mesh improvement algorithms. This increased flexibility allows us to achieve multiple objectives simultaneously where state-of-the-art falls short.

14th U.S. National Congress on Computational Mechanics
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Title: Relaxing the CFL Condition for the Wave Equation on Adaptive Meshes

Author(s): *Roland Maier, Daniel Peterseim, Mira Schedensack, *University of Bonn*.

The Courant-Friedrichs-Lewy (CFL) condition guarantees the stability of the popular explicit leapfrog method for the wave equation. However, it limits the choice of the time step size to be bounded by the minimal mesh size in the spatial finite element mesh. This essentially prohibits any sort of adaptive mesh refinement that would be required to reveal optimal convergence rates on domains with re-entrant corners. This talk shows how a simple subspace projection step inspired by numerical homogenisation can remove the critical time step restriction so that the CFL condition and approximation properties are balanced in an optimal way, even in the presence of spatial singularities. Reference: D. Peterseim and M. Schedensack. Relaxing the CFL condition for the wave equation on adaptive meshes. ArXiv e-print 1601.04812, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: The Shifted Boundary Method for Embedded Boundary Computations

Author(s): *Alex Main, Guglielmo Scovazzi, Nabil Atallah, Ting Song, Kangan Li, *Duke University*.

Embedded boundary methods obviate the need for continual re-meshing in many applications involving rapid prototyping and design. Unfortunately, many finite element embedded boundary methods for incompressible flow are also difficult to implement due to the need to perform complex cell cutting operations at boundaries, and the consequences that these operations may have on the overall conditioning of the ensuing algebraic problems. We present a new, stable, and simple embedded boundary method, which we call “shifted boundary method” (SBM), that eliminates the need to perform cell cutting. Boundary conditions are imposed on a surrogate discrete boundary, lying on the interior of the true boundary interface. We then construct appropriate field extension operators, with the purpose of preserving accuracy when imposing the boundary conditions. We demonstrate the SBM on large-scale incompressible flow problems, multiphase flow problems, and shallow water flow problems.

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Title: Dislocation Dynamics at High Strain-Rate – Inertial and Thermal Effects

Author(s): *Eleanor Mak, Robert Gracie, *University of Waterloo*.

The plastic flow in metals is attributed to the mechanisms of dislocations. Dislocation dynamics (DD) models are characterized by the explicit simulation of discrete dislocations and have been widely used to investigate plastic phenomena at the mesoscale. Due to the heavy computational burden of such simulations, loading rates are often quite high. At such elevated loading rates, both heat generation and inertial effects are important. Conventional DD models are purely mechanical and quasi-static. Here, a fully coupled thermomechanical dynamic DD model implemented within the context of the eXtended Finite Element Method is presented to investigate the strain-rate dependency of material response under high strain-rate loading. Inertial and thermal effects are incorporated, first into an elastodynamic description of the elastic domain response; and second, in the empirical equation governing dislocation motion. A tensile test is simulated into two dimensions to observe the consequence of a dynamic versus a quasi-static implementation, as well as to investigate the sensitivity of the temperature dependence of parameters characterizing dislocation behavior. The impact of inertia on stress-strain response and the evolution of the dislocation system and density is investigated in this simulation framework. The discussion of dynamic effects is extended to a simulation of the nano-indentation of a thin film sample. Sudden bursts of displacement have been observed in load-displacement measurements from experimental trials. The generation and motion of dislocations originating from sources proximate to the contact zone between indenter and film have been suggested as a cause of this response. Dislocation behavior is observed in this setting and rate effects of the loading are investigated. Ultimately, the strain-rate regime where inertial effects become crucial for greater accuracy in the depiction of material behavior is characterized.

14th U.S. National Congress on Computational Mechanics
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Title: A Distributed-Memory Newton-Krylov Solver for Inverse Transport Problems

Author(s): *Andreas Mang, Amir Gholami, George Biros, *University of Texas at Austin*.

We discuss fast algorithms for large scale inverse problems with hyperbolic PDE constraints in three dimensions and their deployment to supercomputing platforms. The PDE constraints of our formulation are the transport equations for a scalar or vector field. The control variable is the velocity field. Our contributions are the following: (i) We present an improved implementation of our memory-distributed, globalized, preconditioned Newton-Krylov solver. (ii) We describe fast schemes to solve the forward and adjoint problems. (iii) We present efficient techniques to precondition the reduced space Hessian. (iv) We study numerical accuracy, rate of convergence, time-to-solution, inversion quality, and scalability of our solver. Inverse transport problems appear in numerous applications in, e.g., geophysical sciences, atmospheric sciences, or medical imaging. They are challenging to solve in an efficient way. They are ill-posed in nature, non-convex and non-linear; they involve an infinite number of unknowns, which-upon discretization-leads to high-dimensional, ill-conditioned, multiphysics systems. Their inversion requires a repeated evaluation of the state and adjoint operators, which are hyperbolic PDEs. The control equation for the velocity is an elliptic integro-differential equation. Our code is implemented in C/C++ and uses the message passing library for parallelism. We use a pseudo-spectral discretization in space. The computational kernels are FFTs and a Semi-Lagrangian scheme with a cubic interpolation model for the time integration of the transport equations. We study the performance of our solver for applications in medical imaging. We report results for a benchmark dataset based on magnetic resonance neuroimaging data. We will see that our solver is competitive with respect to the time-to-solution and outperforms state-of-the-art algorithms in this application domain in terms of the inversion quality. We will see that we can solve problems on clinical images (50 million unknowns) in less than two minutes on a workstation with 40 cores. If we switch to a supercomputing platform we can reduce the time-to-solution to under five seconds, paving the way to tackle real time applications. We will also showcase results for problems of unprecedented scale; we will, e.g., see that we can invert for three billion unknowns in 86 seconds on 2048 cores of TACC's Maverick system.

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Title: Thermal Modelling and Simulation of Selective Laser Melting Additive Manufacturing

Author(s): *Antoinette Maniatty, Souvik Roy, *Rensselaer Polytechnic Inst*; Mario Juha, *Universidad de La Sabana*.

The current leading methods for additive manufacturing of metallic parts are powder bed processes, where successive layers of metal powder are deposited and then melted and fused with either a laser or electron beam. However, these processes often fail to produce acceptable parts due to the high thermal stresses that develop during the build process or due to excess porosity. These issues are associated with the temperature history, phase transformation, and consolidation from powder to dense materials. The complexity of the process makes it both a modeling and simulation challenge. In this work, a novel modified phase field modeling approach is developed and implemented into the high performance computing simulation tool Albany [1] developed by the Computational Multiphysics Department at Sandia National Laboratory, which supports massively parallel simulations. We introduce two state variables into the first law of thermodynamics, a phase parameter to characterize the transition between solid and melt, and a consolidation parameter to characterize the degree of consolidation from powder to dense material. The model is fully implicit allowing for large time steps, and is expressed in a total Lagrangian framework. Furthermore, the laser heating model considers both the heating when the material is powder, including scattering and absorption, and after it has melted and condensed. As the laser beam moves, the mesh is adapted for efficient simulations. Results for simple test cases as well as realistic examples will be presented demonstrating verification and validation. Simple test cases will be used to both show the relationship between the current model and the classic phase field model and to verify the model and implementation for problems with semi-analytic solutions. Examples varying the laser speed, power, and path are shown and the predicted melt zone is compared to experimental results in the literature for validation. [1] https://software.sandia.gov/albany/

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Title: Modeling and Simulation of Residual Stress Development in a Resistance Forge Weld

Author(s): *Kevin Manktelow, *Sandia National Laboratories*.

Resistance welding is a common manufacturing process used to attach a stem to a high pressure vessel. High pressure vessels are complex and expensive to manufacture, so replacing stems on existing pressure vessels for reclamation is of particular interest. The multi-physics elements of the resistance forge weld application problem pose several challenges for current simulation tools. The resistance welding process forms a solid state bond as a result of grain growth and recrystallization across an interface subjected to near-melt temperatures. High temperatures and interference fits required for achieving a solid state weld are also the responsible mechanisms for severe deformations and residual stresses. Cracks along the welded interface have the potential to grow, causing pre-mature pressure vessel failure. Potential crack flaws may be driven by a complex, but unknown, residual stress state following the resistance forge weld and subsequent cooling process. Furthermore, a complex initial stress and material state may already be present before a resistance forge weld even begins. The initial state resulting from material processing and manufacturing steps including initial forging, heat treatments, machining (e.g., the stem from a forging), and cooling all contribute to the final deformation and residual stress state in a non-trivial way that is not well-understood. For example, initial forging and heat treatment process parameters can leave some parts with non-uniform yield strength throughout the body. Hence, the goal of studying the resistance forge weld is to understand many of these complexities through modeling and simulation of the entire manufacturing process. Many of the tools required to solve this class of problem exist already, but procuring a believable result still involves complex physics and numerical solution challenges. The simulation must accurately approximate coupled thermo-mechanical-electrical physics. Joule heating through applied current flux must couple with changing geometry. Heat transfer through all of the necessary mechanisms (conduction, convection, etc.) must be included, along with all of the complexities that go along with discontinuous interfaces (pressure-dependent conduction, mesh tieing, etc.). The solid mechanics portion must deal with rate-dependent and temperature-dependent materials, recrystallization kinetics, resistance weld modeling, and contact at frictional interfaces. This talk describes recent efforts to model the resistance welding process, with an emphasis on consistent remeshing and mapping techniques in a multi-physics environment.

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Title: The Mimetic Finite Difference Method for Elliptic Problems with Staggered Discretizations of Diffusion Coefficients

Author(s): *Gianmarco Manzini, Konstantin Lipnikov, David J. Moulton, Mikhail Shashkov, *Los Alamos National Laboratory*.

We present the new family of mimetic finite difference schemes [1,2] for linear diffusion problems recently proposed in [3]. In contrast to the conventional approach, the diffusion coefficient enters both the primary mimetic operator, i.e., the discrete divergence, and the inner product in the space of gradients. The diffusion coefficient is therefore evaluated on different mesh locations, i.e., inside mesh cells and on mesh faces. Such a staggered discretization may provide the flexibility necessary for future development of efficient numerical schemes for nonlinear problems, especially for problems with degenerate coefficients. These new mimetic schemes preserve symmetry and positive-definiteness of the continuum problem, which allow us to use efficient algebraic solvers such as the preconditioned Conjugate Gradient method. These schemes are inf-sup stable and a priori error estimates are established for the approximation of the scalar and vector solution fields. Numerical examples confirm the convergence analysis and the effectiveness of the method in providing accurate approximations on unstructured polygonal and polyhedral meshes. [1] L. Beirao da Veiga, K. Lipnikov, G. Manzini, "The mimetic finite difference method for elliptic problems", Springer, 2014 [2] K. Lipnikov, G. Manzini, M. Shashkov, "Mimetic finite difference method", Journal of Computational Physics, vol. 257, pages, 1163-1227, 2014 [3] K. Lipnikov, G. Manzini, J. D. Moulton, M. Shashkov, "The mimetic finite difference method for elliptic and parabolic problems with a staggered discretization of diffusion coefficient", Journal of Computational Physics, vol. 305, pages 111-126, 2016

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Title: Modeling Progressive Damage and Fracture of Polymers

Author(s): *Yunwei Mao, Brandon Talamini, Lallit Anand, *MIT*.

The fracture of soft materials has attracted much attention due to the widely applications of the materials. One of the distinguishing features of elastomeric materials is that the deformation response is dominated by changes in entropy. Accordingly, most classical theories of rubber-like elasticity consider only the entropy and neglect any changes in internal energy. On the other hand, the fracture of strongly cross-linked elastomers is essentially energy dominated, as argued in the well-known Lake-Thomas model for the toughness of elastomers. We recently proposed a single model unifying these two phenomena in a paper [2], based on two ingredients: (i) a non-Gaussian statistical mechanics model of polymer chains that accounts for the increase in energy due to the deformation of molecular bonds; (ii) a chain scission criterion based on the bond deformation energy attaining a critical value. Using this model, we can estimate the rupture stretch of elastomeric materials from fundamental quantities describing the polymer network. While this model can address the initiation of the crack propagation, it lacks the ability to tackle the progressive damage and fracture of polymers. A possible way to solve this problem is to use the phase-field method. In the phase-field method, a scalar order-parameter was introduced which can affect the energy storage and stiffness characteristics of the material. Also, with the gradient term of the order-parameter, the traditional Griffith-type theory can be restored. This approach is attractive in its seamless ability to simulate the complicated fracture process of nucleation, propagation, branching and merging of cracks in arbitrary geometries. In this talk we will present the phase-field theory for polymer fracture based on our recent model on rupture of polymers. This theory is developed by using the virtual power approach [1] to make it thermodynamically consistent. We also numerically implemented our theory into a finite element code. Representative numerical examples will be given to show the ability of the simulation capability. Moreover, by including the enthalpy part in the free energy of polymers, we can address a series of interesting problems, and engineer the toughness of soft materials at small scale. This largely extends the capability of the existing model [3]. References: [1] Gurtin, M.E., 1996. Generalizaed Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance. Physica D 92, 178-192. [2] Mao, Y., Talamini, B., Anand L. 2017. Rupture of polymers by chain scission. Extreme Mechanics Letters 13, 17-24. [3] Miehe, C., Schänzel, L-M., 2014. Damage variable modeling of fracture of rubbery polymers. Part I: finite elasticity coupled with brittle fracture. Journal of the Mechanics and Physics of Solids 65, 93-113.

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Title: An Unified Inverse Framework for Identification and Model Updating of Mechanical Structures Involving Non-Linear Behaviors

Author(s): *Basile Marchand, Ludovic Chamoin, *LMT (ENS Cachan/CNRS/UPSaclay)*; Christian Rey, *Safran Tech (Safran Group)*.

Identification and model-updating problems keep receiving a large interest in research and industry. During the last decade, the difficulty came from the evolution of the models used in an industrial context. It is now a standard to perform FEA on industrial structures involving complex behaviors such as visco-plasticity or damage and considering a large number of degrees of freedom. Others applications at a more reduced scale are for example the characterization of delamination in composite materials which requires to use, at the specimen scale alone, a relatively fine mesh. The question according to these evolutions is then how to perform identification and model-updating considering many kinds of behaviors and high dimensional problems. We propose in this talk a general framework (from a theoretical point of view) for the investigation of inverse problems involving non-linear behaviors. This framework is based on the concept of modified Constitutive Relation Error [1] which we extend and generalize using the approach proposed in [2]. In order to solve inverse problems using this formulation, a suitable approach is proposed based on the mathematical properties of the non-linear modified Constitutive Relation Error functional proposed here. This approach leads after development to the LaTIn method [3]. We thus solve alternatively: (i) a linear and global in space problem; (ii) a non-linear but local (at the integration points level) problem. The proposed approach is applied to the identification of damage law parameters characterizing the delamination in a composite material. An industrial model updating application is also addressed considering a visco-plastic behavior and unknown boundary conditions. REFERENCES [1] O. Allix, P. Feissel, H. Nguyen, “Identification strategy in the presence of corrupted measurements”, Engineering, Computations, pp 487-504 (2005). [2] P. Ladevèze, N. Moës and B. Douchin, “Constitutive relation error estimators for (visco)plastic finite element analysis with softening”, Computer Methods in Applied Mechanics and Engineering, pp 246-264 (1999). [3] P. Ladevèze, “Nonlinear computational structural mechanics: new approaches and non-incremental methods of calculation”, Springer, Mechanical engineering series (1999).

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Title: Mesoscopic Modeling of Powder-Bed-Based Additive Manufacturing

Author(s): *Matthias Markl, *University Erlangen-Nuremberg*; Carolin Körner, *University of Erlangen-Nuremberg*.

Powder bed fusion processes are additive manufacturing technologies where components are built up layer by layer in a powder bed by selectively melting con■ned areas, according to sliced 3D model data. This technique allows for manufacturing of highly complex geometries hardly machinable with conventional technologies. Material properties of the resulting components, e.g., density, dimensional accuracy, surface roughness or texture, are complex functions of the material, powder and process parameters. Until today, the exact interplay between these parameters is not fully understood and hardly predictable. This contribution presents mesoscopic numerical modeling approaches to describe different aspects of powder bed fusion processes. We employ a thermal free surface lattice Boltzmann (LB) method, which models the process on the powder scale. In contrast to a continuum approach, this numerical method addresses physical phenomena, like capillary forces, wetting conditions and the local stochastics of individual powder layers. The alloy composition is tracked by a finite difference (FD) approach, where the evaporation of volatile alloy elements is evaluated. Additionally, the grain structure evolution during melt pool solidification is taken into account by a cellular automaton (CA) approach. The numerical simulations elucidate fundamental mechanisms of the underlying physical phenomena. Investigated issues are, e.g., the influence of process parameters, like the beam power, scan velocity or line offset, on, e.g., the formation and quality of walls, the evolution of channel faults bridging through many layers, the density and surface topology of multi-layer hatching, the alloy composition or the grain structure after solidification. In combination with tailored experiments, the numerical results enlarge the process understanding of the underlying physical mechanisms and support the development of suitable process strategies.

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Title: Data-Driven Probabilistic Boundary Layer Model for Prediction of Airfoil Performance

Author(s): Qiqi Wang, *Alexandre Marques, Youssef Marzouk, *MIT*.

In this talk we present a data-driven closure model for the integral boundary layer (IBL) formulation. The IBL is an approximate formulation of the full dynamics of the boundary layer. This formulation is commonly coupled to inviscid flow solvers, resulting in tools that very effective for preliminary airfoil design. Furthermore, the IBL requires a closure model that accounts for the effects of the dynamics that are not resolved by this formulation. We introduce a data-driven, probabilistic model of these unresolved effects for the incompressible and laminar regime. We construct this model by applying supervised learning to a large dataset of boundary layer velocity profiles computed over 1,550 airfoils. The result is a model that (i) is based on a large dataset of realistic airfoil configurations, and (ii) quantifies the model inadequacy associated with the use of an approximate boundary layer formulation. We also create a stochastic version of the airfoil design tool XFOIL by replacing its original boundary layer model with the new probabilistic model. We apply this stochastic version of XFOIL to compute the drag polars of two airfoils at low Reynolds numbers, and compare the results with experimental data.

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Title: Harmonic Balance-Boundary Element Method for 2-D Wave Scattering by a Crack with Contact Boundary Conditions

Author(s): *Taizo Maruyama, Terumi Touhei, *Tokyo University of Science*.

This study deals with nonlinear steady-state 2-D wave scattering by a crack with contact boundary conditions. In general, it is difficult to detect closed cracks under some compressive residual stress by using the conventional linear ultrasonic testing (LUT). This is because the LUT is based on the low-amplitude wave scattering by acoustic impedance mismatch. Underestimation of risk due to this fact is therefore considered as an issue in nondestructive inspection (NDI) for structures and machines. The nonlinear ultrasonic testing (NLUT) based on contact acoustic nonlinearity (CAN) is expected to resolve the problem. Several studies have reported the presence of nonlinear ultrasonic waves which consist of higher- and sub-harmonic components due to the CAN. It has been confirmed theoretically and experimentally that higher-harmonic waves are generated by interaction of crack faces such as clapping motion and dynamic friction (Solodov et al., 2011). However, the theoretical examination of the physical phenomena is not sufficient at present. For instance, the mechanism of sub-harmonic generation is still unclear though it is empirically considered to be associated with resonance of the system containing cracks. In addition, the resonance accompanied with CAN is anticipated to affect higher-harmonic generation significantly. For accurate NLUT, further theoretical investigation of the nonlinear resonance is desirable, and the steady-state analysis is appropriate to the purpose. In this study, a novel numerical method is developed by coupling the boundary element method (BEM) and harmonic balance method (HBM) to investigate the nonlinear steady-state vibration of crack faces. In the proposed formulation, a concept of the nonlinear steady-state vibration of crack faces is introduced as asymptotic behavior of vibration that can be recognized after sufficiently elapsed time. Based on the HBM, the effects of the higher- and sub-harmonic waves are expressed in terms of the Fourier coefficients distributed on crack faces with respect to frequencies. This fact clarifies the details of nonlinear vibration phenomena of crack faces. Several numerical calculations are performed to examine and verify the accuracy of the present formulation. The present numerical results showed almost complete agreement with those obtained by the conventional time-domain BEM. It was also found that the present model reproduces the sub-harmonic generation phenomenon under certain conditions. Reference Solodov, I. Yu., Doring, D., and Busse, G.: New opportunities for NDT using non-linear interaction of elastic waves with defects, Journal of Mechanical Engineering 57, pp.169-182, 2011.

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Title: An Integrated Level Set Methodology for the Generation and Discretization of Complex Heterogeneous RVEs

Author(s): Karim Ehab Moustafa Kamel, *Universite libre de Bruxelles*; Bernard Sonon, *Thierry J. Massart, *Universite libre de Bruxelles* .

The behavior of heterogeneous and/or porous materials is highly dependent of their micro-morphology and their pore spaces morphology. Properties at the micro scale such as pore size and shape distributions and pore network connectivities strongly govern their mechanical, transport and acoustic macroscopic behavior. Models attempting to establish the link between results of experimental observations and the physical understanding of mechanisms into play must thus incorporate explicitly the morphology of studied microstructures. A Representative Volume Element (RVE) of a material can be either obtained experimentally (e.g. CT scans) or numerically generated by algorithms aiming to reproduce its relevant morphological features. In both cases, the RVE geometry must be discretized to simulate its behavior with an appropriate numerical technique such as the Finite Element method (FE). This contribution presents an integrated framework for the generation of RVEs and their subsequent discretization into conforming finite element meshes to conduct multi-scale FE simulations. The implicit representation of the RVEs geometries by level set functions, at the heart of both the RVE geometry and mesh generation procedures, allows for the systematic treatment of morphologies of arbitrary complexity. Previous works by the authors led to the development of an RVE generation methodology using level set functions to implicitly represent and manipulate geometries. It was initially based on a Random Sequential Addition process building packings of arbitrarily-shaped inclusions, controlling neighboring distances using distance fields. It was further extended to more advanced morphologies such as coated and cemented grains assemblies or cellular materials, further working with, and resulting in, level set functions describing the produced geometry. The subsequent mesh generation process is based on a proposition by Persson, using an input level set function to build good quality conforming meshes with a local control of the element sizes, invoking an ad-hoc analogy with the equilibrium of a bar truss. Target bar lengths evaluated from a constructed element size function, and distances from the interface evaluated from the underlying level set function, are used to formulate forces acting on nodes of the truss to steer them to an equilibrated situation, satisfying conformance of the mesh with material interfaces as well as controlling element sizes, while ensuring a very good shape factor for elements. This approach has been extended here for the case of the multi-body geometries of complex RVEs and will be illustrated with both computationally generated RVEs and on real samples obtained from CTX scan.

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Title: CutFEM: Discretizing Geometry and Partial Differential Equations in Multidimensional Multiphysics Problems

Author(s): *André Massing, Mats G. Larson, *Umeå University*; Erik Burman, *University College London*; Peter Hansbo, *Jönköping University*.

We consider a cut finite element framework [1] for the numerical solution of partial differential equations (PDEs) posed on and possibly coupled through domains of different topological dimensionality. Important examples include the modeling of flow and transport in porous media with large-scale networks of fractures and channels, reaction-diffusion systems to describe cell motility or two-phase flow problems with surfactants. To allow for a flexible discretization and easy coupling between PDEs in the bulk and on lower dimensional manifold-type domains, the lower-dimensional geometries are embedded in an unfitted manner into a three dimensional background mesh consisting of tetrahedra. Since the embedded geometry is not aligned with the background mesh, we use the trace of finite element functions defined on the tetrahedra in the discrete formulations. As the resulting linear system may be severely ill-conditioned, we discuss several possibilities for adding (weakly) consistent stabilizations terms to the original bilinear form. We present an abstract CutFEM framework which allows us to treat PDEs on embedded manifolds of co-dimension >= 1 (see [2]) and multi-dimensional coupled problems in a unified manner. Starting from a few abstract key assumptions which leads to provably optimally convergent and geometrically robust CutFEM schemes, we discuss a number of possible CutFEM realizations. In particular, the general mechanism behind current CutFEM stabilizations is highlighted, including the classical face based stabilization, a simple full-gradient based stabilization and finally a novel normal-gradient based stabilization which is suitable for higher-order approximations of surface PDE problems. Along with presentation of the framework we give a number of numerical examples illustrating the theoretical findings and the applicability of the framework to complex modeling problems. In particular, we present a novel stabilized CutFEM for the Darcy surface problems building upon the classical Masud-Hughes formulation [3] and applications to surface-bulk problems related to modeling of porous media. [1] Burman, E. and Claus, S. and Hansbo, P. and Larson, M. and Massing, A. CutFEM: discretizing geometry and partial differential equations. Int. J. Numer. Meth. Engng. 104:472– 501 (2015). [2] Burman, E. and Hansbo, P. and Larson, M. and Massing, A. Cut Finite Element Methods for Partial Differential Equations on Embedded Manifolds of Arbitrary Codimensions. arXiv:1610.01660 (2016). [3] Masud, A. and Hughes, T.J.R. A stabilized mixed finite element method for Darcy flow. Comput. Methods Appl. Mech. Engrg. 191 39:4341-4370 (2002).

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Title: Variational Interfacial Coupling in Thermo-Mechanical Field Problems at Finite Strains

Author(s): *Arif Masud, *University of Illinois at Urba*; Pinlei Chen, *University of Illinois at Urbana-Champaign*.

Many problems in engineering and sciences involve multiple simultaneous physical phenomena, each governed by their own balance laws and constitutive models, and therefore associated material, spatial and temporal scales. This talk presents new developments in multi-model interface framework by embedding Discontinuous Galerkin (DG) ideas in the Continuous Galerkin (CG) method within the context of Stabilized Methods. Starting from a thermo-mechanically coupled formulation, a Lagrange multiplier method along the interface is developed. Employing ideas for VMS based stabilization, the interfacial fine-scale problem is expended via edge bubbles and resolved locally to extract an analytical expression for Lagrange multipliers. The derived expression is a function of evolving mechanical and thermal fields and therefore the derived stabilized formulation contains the numerical flux and stability tensor which are free from user-defined parameters. The coupled thermomechanical method is applied to interface problems with strong discontinuities such as debonding at the fiber matrix interface due to both thermal and mechanical effects. The evolution of the debonding parameter is modeled through internal variables such as an inelastic gap at the interface. Several test cases are presented to validate the method. The method is applied to model engineered materials governed by a spectrum of isotropic and anisotropic constitutive equations in the finite strain range to illustrate its versatility and applicability.

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Title: Combat Helmet Design Incorporating Anthropomorphic Fit, Brain Functional Areas and Injury Considerations

Author(s): Robert Saunders, Xiangguang (Gary) Tan, *Peter Matic, *Naval Research Laboratory*.

Combat helmet parametric design strategies are implemented in a computer aided design (CAD) software application. The application evaluates 3000 ballistic impact origination points, each directed at 104 representative brain points; the helmet material and geometric parameters; and a standard set of common head impact brain injuries. Performance is expressed in terms of helmet coverage, back face deflection (BFD) and head-helmet system impact-induced motion. Application speed, sufficient for convenient and iterative design studies, is achieved in a desktop computer environment by using a set of direct calculations, first-order models and tabulated empirical data. The analysis results define the helmet trade space, facilitate prototyping and support helmet design optimization. This presentation focuses on (i) using the CAD application to compare performance of four notional helmet designs using recent anthropomorphic dimensional data to a standard military helmet and (ii) strategies combining ballistic impact physical tests and computational simulations to efficiently generate ballistic resistance and BFD data for the CAD application. The head-to-helmet spacing distribution, calculated by the CAD application using a standard military helmet and anthropomorphic dimensional data from a relevant military population, has potential implications for helmet BFD injuries. Helmet geometries designed to generate a more uniform spacing with the anthropomorphic data were evaluated by the application. The predicted deformation and injury results for the anthropomorphic helmet were compared to the baseline helmet quantifying the trade-offs between head coverage, head-to-helmet spacing, and BFD injuries. The CAD software application speed is based on the models employed. Ballistic material test data is a requisite for modeling, generally acquired at high cost with long lead times. Finite element analysis provides cost effective insight with validated models. Appropriate combinations of physical testing and computational simulation can optimize data generation and essential insight. Building on prior experimental work, using flat panels of helmet ballistic materials, pad suspensions, skull bone simulants and brain tissue simulants, parametric simulations were conducted for combinations of threats, impact obliquity and strike velocity. The non-penetrating ballistic damage and deformation of thick-section aramid fabric composite laminate was solved utilizing a progressive composite damage model to predict the initiation and evolution of different composite damage modes. Model validation against ballistic experiments was performed to determine rate sensitive model parameters. The strain-rate dependent material model based on the tabulated approach was used for the pad suspension. Results from the validated model were used to construct BFD and the acceleration-time curves to support the helmet CAD application.

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Title: Integrated Computational Materials Engineering

Author(s): *Karel Matous, *University of Notre Dame*.

With concentrated efforts from the material science community to develop new multi-functional materials using unique processing conditions, the need for modeling tools that accurately describe the physical phenomena at each length scale has only further been emphasized. For example, additive manufacturing and shock synthesis lead to unique material morphologies that need to be understood for reliable engineering analysis and product safety assessments. Considering these material complexities, Direct Numerical Modeling (DNM) is accessible only for moderate system sizes. Thus, a multiscale strategy must recognize that just a relatively small part of the material will typically be instantaneously exposed to rapid material transformations. Macroscopic constitutive models obtained from homogenization, of the complex but slowly varying microstructure, may adequately describe the rest of the material. Nonlinear model reduction, pattern recognition and data-mining are a key to future on-the-fly modeling and rapid decision making. To address these challenges, we present an image-based (data-driven) multiscale framework for modeling the chemo-thermo-mechanical behavior of heterogeneous materials while capturing the large range of spatial and temporal scales. This integrated computational approach for predicting the behavior of complex heterogeneous systems combines macro- and micro-continuum representations with statistical techniques, nonlinear model reduction and high-performance computing. Our approach exploits the instantaneous localization knowledge to decide where more advanced computations are required. Simulations involving this wide range of scales, O(10^6) from nm to mm, and billions of computational cells are inherently expensive, requiring use of high-performance computing. Therefore, we have developed a hierarchically parallel high-performance computational framework that executes on hundreds of thousands of processing cores with exceptional scaling performance. Any serious attempt to model a heterogeneous system must also include a strategy for constructing a complex computational domain. This work follows the concept of data-driven (image-based) modeling. We will delineate a procedure based on topology optimization and machine learning to construct a Representative Unit Cell (RUC) with the same statistics (n-point probability functions) to that of the original material. Our imaging sources come from micro-computed-tomography (micro-CT), focused ion beam (FIB) sectioning, and advanced photon source nano-tomography at the Argonne National Laboratory. We show that high-performance DNM of these statistically meaningful RUCs coupled on-the-fly to a macroscopic domain is possible. Therefore, well-resolved microstructure-statistics-property (MSP) relationships can be obtained.Finally, the integrated V&V/UQ program with co-designed simulations and experiments provides a platform for computational model verification, validation and propagation of uncertainties.

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Title: Nonlinear Dynamic Analysis of Shell Structures

Author(s): *Takuya Matsumoto, Shigenobu Okazawa, *University of Yamanashi*.

We present a nonlinear dynamic analysis of shell structures such as in the case of buckling and collapse. Solving this buckling and collapse behavior is crucial for automoblle crash analysis. In this presentation, after describing the computational theory of large deformation and rotation shells, we test the dynamic stability performance.

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Title: qADMESH+: An Automatic Quadrangular and Mixed-Element Mesh Generator

Author(s): *Dominik Mattioli, Ethan Kubatko, *The Ohio State University*; Alan Zundel, *Aquaveo - Water Modeling Solutions*.

In this talk, we introduce a new automatic mesh generator that creates a high quality, unstructured, quadrilateral/mixed-element mesh given a pre-existing, unstructured, triangular mesh. A primary motivation of this work is to provide a mesh-generating tool that may be used in modeling shallow water flow within a Discontinuous Galerkin (DG) finite element framework - a setting where meshes of mixed-element composition are easily accommodated and demonstrably advantageous. Some of the employed techniques in our approach include the following: A triangular mesh generation algorithm ADMESH+; an innovative and strategic matching sequence that merges triangular elements together to form quadrilaterals; a supplemental corrective routine on elements along domain boundaries; several topological improvements designed to improve quality of elements in the resultant mesh; and a smoothing method.

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Title: Immersive Simulation of the Reduction of Femoral Diaphyseal Fracture

Author(s): *Mohamed Mediouni, Djemel Ziou, François Cabana, *Université de Sherbrooke*.

With the advancement of the virtual technologies, three-dimensional surgical simulators are now possible. In this article, we describe an immersive simulation platform, allowing students in orthopedic surgery to learn how to deal with a sample diaphyseal fracture of the femur using LC-DCP plate hole, cortical screw and verbrugge forceps. To reach certain realism, weight of the objects and force feedback are used in addition to the visual scene and the 3D sound. The students feel the weight, the strength of the bone when they pierce the holes, and the vibration of the drill. The simulation is implemented by using CAVE, the CyberGlove, CyberGrasp, and 3D sound system.

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Title: Modeling Blast Loading on Structures from Explosions in an Urban Environment

Author(s): *Sergey Medyanik, *MES*; Syed Mohammad, *HQ DHS S&T, CDS ORA*; Nickolas Vlahopoulos, *University of Michigan*.

Full size physical tests of blast events are very expensive and difficult to organize. Even if properly implemented, such tests may only explore a limited number of options and parameters. Using numerical simulations, such as finite element method, provides an alternative approach for modeling the effects of explosions on building and other structures which allows for quick and reliable assessment for a wide range of geometric configurations, explosive materials, structural parameters, and other options. The general goal of the current work is to develop a proper procedure for assessing the loads induced on buildings due to pressure waves originating from explosions as well as estimating the resulting damage and finding the ways of reducing it. The general procedure consists of two main steps. First, the loads induced on structures from the explosion are evaluated using Eulerian simulation approach. Then, the calculated loads can be applied to structures for Lagrangian structural analysis, which may be repeated several times in order to study the resulting damage and how the blast worthiness of buildings can be improved. This presentation will focus on the first part of the project, which consists in evaluating the existing numerical methods capabilities for modeling blast events regarding their accuracy and general applicability for the current project. In particular, several typical geometric configurations will be considered. First, blast pressure on a free standing structure due to explosion will be calculated and compared to experimental data. Then, a series of numerical simulations will be performed for a number of street configurations that are typical for an urban environment. Special effects, such as reflected shock and channeling effects, which occur due to confinement between the walls of buildings in urban city centers, will be investigated. In addition, mesh sensitivity of the results and a proper choice of meshes for various explosion stand-off distances will be examined. The simulation results will be verified by comparing to the existing experimental data.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Modelling Powder Bed Fusion Feature Creation

Author(s): Wolgang Ottow, *Mustafa Megahed, *ESI Group*.

Modelling powder bed fusion processes involves resolution of several interacting physical phenomena. Laser irradiation is a key phenomenon driving powder heat up, melting and eventually the solidification of consolidated material. The thermal history of the work piece is usually complex both in space and time. The material shrinkage and clamping devices lead to residual stresses that affect the final work piece shape. The final work piece properties, the accumulated residual stresses and the overall distortions are complex functions of the input parameters: Powder and heat. Due to the complex physics encountered in powder bed fusion processes researchers sought to analyze single aspects of the manufacturing process. A group of researchers focused on radiation aspects of the problem, others focused on melt pool dynamics and A larger group of researchers focus on work piece distortion. The resolution of the heat source track in a fully transient manner requires massive computational resources. The calculation of the work piece distortions is thus pursued using simpler models such as inherent plastic strain. There has been very little transfer of information from high fidelity models to large scale models resolving work piece residual stresses and distortion. This presentation will introduce a multi-scale multi-physics platform that resolves the powder coating process, the heat source absorption, material phase changes (melting, evaporation and solidification), defects related to powder bed spreading and material consolidation as well as residual stress and distortion predictions. Verification and validation studies published in the past will be briefly touched upon before presenting detailed analysis of phenomena and processing steps taking place during laser based powder bed fusion of an L shaped structure: The powder is spread numerically starting with a smooth processing table. The powder particles are then molten using a laser to create a planar feature geometry. The consolidated material is cooled down to obtain the new geometry after shrinkage. A new layer of powder is spread on the processed material, the laser scanning direction is rotated and so on. The manufacturing process is repeated numerically several times. The transfer of data between scales is performed for each layers providing the first closed loop ICME analysis of a geometric feature. The results are analyzed for each step and layer providing insight on how the powder coating is affected by material consolidation, the quality of solidified layers and the microscopic stresses generated during solidification.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Parallel Numerical Methods for Black-Box Coupling in Surface Coupled Multi-Physics Problems and Beyond

Author(s): *Miriam Mehl, Klaudius Scheufele, Florian Lindner, *University of Stuttgart*; Benjamin Uekermann, *Technical University of Munich*.

For the simulation of complex scenarios in engineering and sciences, not only a very high computational power and efficiency is required to achieve the required accuracy, but also oftentimes several existing black-box components have to be combined in a coupled simulation environment to provide a software solution for a new setting in acceptable development time. Throughout the last years, we have developed preCICE, a comprehensive library for surface-coupling of black-box solvers in multi-physics applications, i.e., scenarios, where different sets of equations interact at a common surface (lower dimensional manifold) in the computational domain. A prominent example is the simulation of fluid-structure interactions. In preCICE, we implemented all three technical and numerical components involved in surface coupling: a highly efficient and scalable point-to-point communication between the processes of the involved (parallel) single-physics solvers that comes without a central server as potential bottleneck; several options for data-mapping between the in general non-matching meshes of the solvers at the coupling surface, one of them, the radial basis function method with several optimizations introduced towards better conditioning, parallel scalability, and usability even suited for surfaces meshes given by plain clouds of data points instead of meshes; various variants of quasi-Newton solvers for the interface equations arising from implicit surface coupling in every time step. The latter is required for physically strongly coupled problems in order to ensure stability of the time stepping. We introduced several new variants that feature linear complexity in the number of interface unknowns, high parallel scalability, and robustness in terms of parameter choices. We have shown the applicability of preCICE for various scenarios including fluid-structure interactions, but also multi-field interactions and fluid-acoustics simulations. We present novel optimzations of all coupling components implemented in preCICE and numerical, performance and scalability results for various coupled simulation scenarios. [1] Bungartz, Hans-Joachim; Lindner, Florian; Gatzhammer, Bernhard; Mehl, Miriam; Scheufele, Klaudius; Shukaev, Alexander; Uekermann, Benjamin: preCICE – A Fully Parallel Library for Multi-Physics Surface Coupling. In: Computers & Fluids, Elsevier, 2016. [2] Bungartz, Hans-Joachim; Klimach, Harald; Krupp, Verena; Lindner, Florian; Mehl, Miriam; Roller, Sabine; Uekermann, Benjamin: Fluid-Acoustics Interaction on Massively Parallel Systems. In: Mehl, Miriam (Hrsg); Bischoff, Manfred (Hrsg); Schäfer, Michael (Hrsg): Recent Trends in Computational Engineering, Berlin, Heidelberg, New York: Springer, 2015. [3] Bungartz, Hans-Joachim; Lindner, Florian; Mehl, Miriam; Uekermann, Benjamin: A plug-and-play coupling approach for parallel multi-field simulations. In: Computational Mechanics. Vol. 55(6), Berlin, Heidelberg, New York: Springer, 2015.

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14th U.S. National Congress on Computational Mechanics
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Title: Geometrically Exact Finite Element Formulations for Slender Beams: Kirchhoff-Love Theory vs. Simo-Reissner Theory

Author(s): *Christoph Meier, *Massachusetts Institute of Technology*; Wolfgang A. Wall, Alexander Popp, *Technical University of Munich*.

Highly slender fiber- or rod-like components represent essential constituents of mechanical systems in countless fields of application. Examples are high-tensile industrial ropes and webbings, fiber-reinforced composite materials or synthetic polymer materials. On entirely different time and length scales, such slender components are relevant when analyzing the supercoiling process of DNA strands, the characteristics of carbon nanotubes or the Brownian dynamics within the cytoskeleton of biological cells. In this contribution, finite element formulations for the modeling of such highly slender mechanical members are proposed on the basis of the geometrically exact Kirchhoff-Love beam theory. Compared to other classes of geometrically nonlinear beam elements, geometrically exact beam element formulations are characterized by a highest degree of accuracy and computational efficiency. While the existing representatives are almost exclusively based on the Simo-Reissner theory of shear-deformable beams [1], the current work proposes novel finite elements based on the geometrically exact Kirchhoff-Love theory of thin beams [2,3]. The proposed formulations are the first of this category that account for curved 3D initial geometries with anisotropic cross-section shapes and fulfill the fundamental mechanical properties of objectivity and path independence. For finite elements derived from 3D Boltzmann continua such properties are standard. However, the non-additivity and non-commutativity of the configuration space underlying geometrically exact beams, which can be identified as a nonlinear manifold with Lie group structure, requires special interpolation strategies. Thereto, novel orthonormal rotation interpolation schemes are proposed that eventually yield two alternative beam elements based on a strong and a weak enforcement of the Kirchhoff constraint, respectively. It is shown that these finite element formulations offer considerable numerical advantages in the range of high beam slenderness ratios as compared to the existing counterparts of Simo-Reissner type. As an example, the accumulated number of nonlinear iterations could be reduced by up to two orders of magnitude in the high slenderness regime. [1] J. C. Simo, A finite strain beam formulation. The three-dimensional dynamic problem. Part I, Computer Methods in Applied Mechanics and Engineering 49, 55–70, 1985. [2] C. Meier, A. Popp and W. A. Wall, An objective 3D large deformation finite element formulation for geometrically exact curved Kirchhoff rods, Computer Methods in Applied Mechanics and Engineering 278, 445–478, 2014. [3] C. Meier, W. A. Wall and A. Popp: Geometrically exact finite element formulations for slender beams: Kirchhoff-Love theory vs. Simo-Reissner theory, submitted for publication.

14th U.S. National Congress on Computational Mechanics
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Title: Out-of-Plane Deformation Behavior of 3D Graphene Honeycomb Structures: Atomistic Simulations and Continuum Modeling

Author(s): *Fanchao Meng, Jun Song, *McGill University*.

Understanding of the structure-property relationships is key to designing 3D nanostructures assembled from 2D nanomaterials. Combining atomistic simulations and continuum modeling, this work studied the out-of-plane compression behavior of two types of 3D graphene honeycombs of various honeycomb prism side length (l), namely ac-sp2 and zz-sp2sp3 honeycombs with the major difference lying in their sp2- and sp3-bonded structural junctions, respectively. Interestingly, for the same l, ac-sp2 honeycomb possesses both higher critical buckle stress than that of zz-sp2sp3 honeycomb and a unique hexagonal to orthorhombic structural transformation, while the fracture strength remains nearly the same for both. Following continuum elasticity theory, the simulated critical buckle stress for the zz-sp2sp3 honeycombs can be well predicted. On the other hand, a new model was proposed to quantify the buckling stress of the ac-sp2 honeycombs to account for the excessive strain energy absorbed by the sp2-bonded junction, which subsequently leads to the structural transformation. Nearly the same fracture strength of both types of honeycombs can be attributed to the fact that fracture initiates from the honeycomb wall, i.e., essentially graphene for both honeycombs. Furthermore, buckle stress and fracture strength are highly dependent on l that should be treated as a critical factor for the 3D nanostructures design. Our study integrates multiscale modeling techniques to provide critical insights into structure-mechanical properties relationships and rational design of 3D nanostructures.

14th U.S. National Congress on Computational Mechanics
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Title: A Laminate-Based Computational Model for Ferroelectric Single Crystals and Ceramics

Author(s): *Andreas Menzel, Dinesh Dusthakar, *TU Dortmund*; Bob Svendsen, *RWTH Aachen*.

The present contribution deals with the development of a laminate-based model in order to study single crystal and polycrystalline ferroelectric material behavior. Laminate-based models are micromechanically motivated and directly include the volume fraction of distinct ferroelectric variants in the model formulation. At first, a single crystal laminate-based model is established by considering the average strain and polarization compatibility conditions. A suitable thermodynamic electric Gibbs energy and a scalar rate-dependent dissipation equation are postulated to capture the dissipative hysteretic material response. The update of the inequality constrained evolution of the volume fractions is solved by a Fischer-Burmeister-type algorithm in combination with a Newton-Raphson scheme. Following the single crystal formulation, a random orientation of the individual grains in a polycrystalline aggregate is considered. Related inhomogeneous boundary value problems are solved in the context of the finite element method. Representative material properties and the polarization switching response of the randomly oriented individual grains are averaged within the finite element formulation established in order to study the macroscopic polycrystalline behavior. Finally, a parameter fitting procedure based on available experimental data is detailed and the material model as well as the algorithmic scheme are discussed by representative boundary value problems. D. Dusthakar, A. Menzel, B. Svendsen. Comparison of phenomenological and laminate-based models for rate-dependent switching in ferroelectric continua. GAMM-Mitteilungen, 38(1):147-170, 2015, DOI: 10.1002/gamm.201510008. B. Kiefer, T. Bartel, A. Menzel. Implementation of numerical integration schemes for the simulation of magnetic SMA constitutive response. Smart Materials and Structures, 21(9):094007, 2012. J.-H. Yen, Y.-C. Shu, J. Shieh, J.-H. Yeh. A study of electromechanical switching in ferroelectric single crystals. Journal of the Mechanics and Physics of Solids, 56(6):2117-2135, 2008.

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Title: Computational Modeling of Fluid Induced Fracture Propagation: XFEM and Variational Interface Methods

Author(s): *Gunther Meschke, Ildar Khisamitov, Dirk Leonhart, Beckhuis Sven, *Ruhr University Bochum*.

The hydraulic stimulation of deep geothermal reservoirs is characterized by the creation of hydraulically driven fractures, which eventually interact with pre-existing fractures and natural faults. In the presentation, two computational modelling strategies formulated in a coupled poromechanics framework are discussed: The first model is based on a coupled poroelastic Extended Finite Element (XFEM) model, which uses suitable enrichment functions to model crack tips as well as the coalescence of fractures. The capability of this model to capture the interaction of complex fracture networks is demonstrated. The second modeling strategy is based on a novel variational approach to model brittle fracture propagation using zero-thickness elements. The fractured structure is variationally formulated as the sum of bulk elastic and fracture surface energies. With the help of a damage variable used as an additional degree of freedom, the fracture propagates according to a minimization principle of the total potential energy. As a criterion for the crack propagation, an energy criterion, checking, if the elastic energy within the interface surface exceeds the critical energy release rate is used. Alternatively, a stress criterion is employed. Equilibrium of the discretized structural boundary value problem is found using a staggered scheme, solving first the mechanical problem and then searching for the solution for the updated damage variable. Besides selected benchmark tests, also various laboratory tests fluid induced fracture propagation are analyzed numerically and compared with the experimentally obtained fracture path.

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14th U.S. National Congress on Computational Mechanics
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Title: On Dynamic Load Balancing Schemes for Adaptive Finite Element Solvers

Author(s): *Youssef Mesri, Elie HACHEM, *MINES-ParisTech*.

This work is motivated by the success of the anisotropic adaptive finite element methods in accurately simulating complex physical systems in science and engineering. The parallel implementation of anisotropic adaptive finite element methods is a challenging task for which load imbalance continue to be a significant bottleneck in the global simulation efficiency. We have developed and optimized in the last years, tools and algorithms to manage efficiently the dynamic load balancing in the framework of parallel anisotropic mesh adaptation [1, 3]. However, there still complicated and challenging to predict a quantified estimation of parallel workload of adaptive finite element meshes. Indeed, the mesh adaptation procedure changes dynamically the size of the mesh over all the processes. This mechanism is managed by an anisotropic error estimator that allows to equi-distribute the error over the entire domain by refining and coarsening the mesh in the regions where it is needed [2]. In other words, the size of the problem changes permanently along the runtime execution. The leading questions that arise from this analysis are: how to derive a scalability model to measure the parallel efficiency of a dynamic adaptive simulation? And how to estimate quantitatively the worakload needed to achieve the remeshing stage? We propose in this paper, an anisotropic a posteriori error estimator that controls the error due to mesh discretization in all space directions. From the a posteriori error analysis, we get an optimal metric (optimal mesh) as a minimum of an error estimator function constrained by a given number of elements. The optimal metric obtained is used to build an optimal mesh for the given number of elements and also to derive a quantitative estimation of the work that will be done in the remeshing stage. We conduct performance analysis over different multi-phase flows [4] to highlight effectiveness of the proposed approach. REFERENCES [1] Y. Mesri, H. Digonnet, T. Coupez. Advanced parallel computing in material forming with CIMLib. E. J. of Computational Mechanics, 18(7-8):669-694, 2009. [2] Y, Mesri, M. Khalloufi, E. Hachem, On optimal simplicial meshes for minimizing the Hessian-based errors, APNUM, Vol. 109, pp. 235-249, 2016 [3] Y. Mesri, H. Digonnet, T. Coupez, Hierarchical adaptive multi-mesh partitioning algorithm on heterogeneous systems. Parallel Computational Fluid Dynamics 2008, 299-306 [4] E. Hachem, M. Khalloufi, J. Bruchon, R. Valette, Y. Mesri, Unified adaptive Variational MultiScale method for liquid-gas flows, Computer Methods in Applied Mechanics and Engineering, Vol. 308, pp. 238-255, 2016

14th U.S. National Congress on Computational Mechanics
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Title: Advances in Algebraic Multigrid (AMG) for the Finite Pointset Method (FPM)

Author(s): *Bram Metsch, Fabian Nick, *Fraunhofer SCAI*.

Algebraic multigrid (AMG) methods provide robust and scalable linear solvers for a wide class of sparse linear systems arising from the discretization of partial differential equations. In contrast to classical (one-level) iteration schemes like the conjugate gradient or GMRES method, they only require linear compute time with respect to the problem size. The key idea of multigrid methods is to deal with different frequencies of the underlying problems on different "grids". To this end, a multi-level hierarchy of linear systems is needed. While in geometric multigrid this hierarchy needs to be given by the user, algebraic multigrid methods automatically construct the hierarchy using the initial linear system matrix. In particular, AMG does not require a "grid" or a "mesh" and hence is well suited for mesh-free methods. While initially developed for symmetric positive definite matrices (as they typically arise in finite difference, finite element and finite volume discretizations of scalar elliptic PDEs), AMG methods have been successfully employed also beyond this class. Depending on the application, this requires modifications to the original AMG hierarchy construction. In this talk we describe recent developments of AMG for the Finite Pointset Method (FPM), a mesh-free generalized finite difference method for continuum mechanics. We focus on the matrices evolving from the FPM discretization of the Navier-Stokes equations, which comprises pressure systems, three-dimensional velocity systems, and coupled velocity-pressure saddle point systems. For each of these, we present suitable AMG techniques and illustrate their robustness in several numerical examples. (This is joint work with the Grid-free methods group at Fraunhofer ITWM.)

14th U.S. National Congress on Computational Mechanics
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Title: Modelling of Nanoscale Phononic Crystals

Author(s): *Ralf Meyer, *Laurentian University*.

Phononic crystals are artificially structured materials that use Bragg reflection to control the propagation of elastic waves. Phononic crystals have potential applications in areas such as noise control, ultrasound imaging, wireless communication and thermal management in nanodevices. Nanotechnology makes it possible to produce phononic crystals that operate on the wavelengths of the lattice vibrations responsible for heat transport in insulating materials. Such phononic crystals are candidates for thermoelectric materials with high figures of merit ZT which may be used to transform waste heat into electricity. The modelling of nanoscale phononic crystals for wavelength in the nanometer range is a challenging task. Phononic crystals operating on longer wavelengths can be modelled effectively with continuum methods. On the nanoscale, however, additional effects not captured by the continuum approach influence the properties of materials. These nanoscale effects are typically caused by surfaces and interfaces or the discrete nature of the crystalline lattice of atoms.Such effects are automatically included in atomistic molecular dynamics simulations. The modelling of phononic crystals require, however, large scale simulations with tens of millions of atoms over periods of nanoseconds. In this presentation, results will be shown from both molecular dynamics simulations of a phononic crystal as well as from finite element computations of a simplified continuum model [1]. The vibrational band structure of the simulated crystal has been derived from the molecular dynamics simulations. The results agree qualitatively very well with the band structure obtained from the finite element computations. A slight improvement of the continuum model leads to further improvements of the agreement. The goal of this project is to use molecular dynamics simulations to study the impact of specific features of a nanostructure (e.g. interface or grain boundaries) on the vibrational properties. The results from the simulation will then be used to improve the continuum model (e.g. through the addition of specific surface or interface terms) so that it can account for the nanoscale effects. The continuum model can then be used to simulate and study much larger and more complex structures, e.g. acoustic diodes. [1] R. Meyer, Phys. Status Solidi A 213, 2927 (2016).

14th U.S. National Congress on Computational Mechanics
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Title: Modeling Contact Interfaces by Considering Structural Anisotropy and Plasticity

Author(s): *Georgios Michaloudis, Norbert Gebbeken, *Univ. of the Bundeswehr Munich*; Alexander Konyukhov, *Karlsruhe Institute of Technology*.

Interfaces between different materials occur in several engineering applications. The characteristics of these interfaces depend on the local geometry as well as on the material parameters of the adjacent surfaces. The numerical modeling of these systems requires a robust description of the interface and of the interaction of the different materials, especially under loading conditions leading to large deformations. This contribution addresses the formulation and implementation issues of interface finite elements suitable for the modeling of contact interfaces. The formulation of the elements is based on a general three-dimensional contact formulation which is derived within a fully covariant approach. This formulation is then enriched with an appropriate material law for the description of the tangential interaction of the materials. The material law is derived as a "load-relative displacement" interface model resulting from suitable experiments and assumes plastic deformations. The proposed model is further developed in order to consider structural anisotropy on arbitrary surfaces. Starting from the principle of maximum dissipation we derive an appropriate "Return-Mapping" algorithmic scheme in order to compute the correct contact traction in each time step for both the isotropic, see [1], and anisotropic case. The description of the sticking/elastic region is anisotropic, which allows to describe the structure of the surface, while the plastic region remains isotropic. The isotropic formulation is validated through experimental results, whilst the anisotropic through analytical solutions. The effect of structural anisotropy on the kinematic behavior of contacting bodies is shown in numerical examples. By substituting the widely used Coulomb friction law with the proposed associative plasticity model we derive a symmetrical stiffness matrix of the tangential contact for "sticking" as well as for "sliding", since the non-associative nature of the Coulomb law is abandoned. In this way a general frictional contact formulation is presented, appropriate for the numerical modeling of arbitrary interface phenomena. [1] G. Michaloudis, A. Konyukhov, N. Gebbeken. An interface finite element based on a frictional contact formulation with an associative plasticity model for the tangential interaction. Int. J. Numer. Meth. Engng (2017) Published online. DOI: 10.1002/nme.5485

14th U.S. National Congress on Computational Mechanics
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Title: Effective Thermal and Elastic Properties of a Composite with Spheroidal and Ellipsoidal Inhomogeneities

Author(s): *Yozo Mikata, *Bechtel*.

This presentation will discuss the effective material properties of a composite with spheroidal and ellipsoidal inclusions and voids. The method is based on Eshelby's equivalent inclusion method. Both dilute approximation and Mori-Tanaka's method will be discussed for oblate and prolate spheroids, and general ellipsoids whose orientation is either aligned or completely random. Analytical formulations and numerical results will be given. In numerical results, all the constituents are assumed to be isotropic.

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Title: Multiphysics Modelling of Very Low Flow Rate Micropump Based on Thermal and Mechanical Actuation

Author(s): Hamza Landari, *Laval university*; *Amine Miled, *Université Laval*.

Liquid control at extreme low flow rate is still not well established in terms of the system level design. This is mainly due to challenges and difficulties in the design of an extremely highly sensitive actuator to control liquid flow. Such systems may be very useful for drug delivery at the microscale. But it requires advanced, expensive and time consuming microfabrication process. Then, modeling becomes critical step at this stage. However, such system is a hybrid and multiphysics integration between structural and/or thermal and/or fluidic at least. In this work we present the numerical modeling and associated challenges of a low flow-rate micropump with integrated microvalve. Modeling of the proposed micropump was achieved with ANSYS Multiphysics. We used the transient structural module to estimate the maximum deformation of the membrane caused by the external pressure. '' Fluid Flow (Fluent) '' was also used to model the flow and calculate the pressure induced by a membrane deformation. We used a standard meshing for the structural part with a meshing refinement on the boundaries in contact with the fluid. Regarding the fluidic part of the model, we fixed a fine mesh everywhere with dynamic meshing. Model operations consist of two phases: infusion phase where a membrane deformation takes place by increasing the volume of the pumping chamber and creating a spherical cap and thereafter decreasing the pressure in the pumping chamber. Then the fluid will move to the pumping chamber in order to reach a dynamic equilibrium of the pressure in different area of the micropump. Embedded valves close the inlet and opens the outlet and vice versa. During the infusion phase, the vacuum created in the pumping chamber induces a deformation of the valve diaphragm to close the outlet channel. The other phase of operation is the withdraw phase where the membrane deformation takes place in the other direction to decrease the volume of the pumping chamber. The latter increases the pressure in the pumping chamber and it also applies a reverse pressure on the valve to reverse the deformation and open the outlet channel. All simulation step were 1/10 * period, membranes and valves are made with PDMS. The thickness of the membrane is equal to 440 μm, the radius of the micropump was 13.5 mm. Inlet and outlet port inner surface was 0.38 mm2. The deformation of the actuation membrane was 0.32 μm.

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Title: Numerical Investigation of Iterative Coupling for Structural Acoustics

Author(s): *Scott Miller, Gregory Bunting, *Sandia National Laboratories*.

Partitioned versus monolithic coupling for FSI simulations is a topic that continues to receive attention. In this work, we numerically investigate the accuracy and computational costs of a partitioned coupling algorithm for structural acoustics. The acoustic and structural subdomains are both solved implicitly using Sierra/SD, and the partitioned coupling is accomplished through the use of an MPI-based, multiple program multiple data (MPMD) implementation. Results obtained from the partitioned methods are then compared to a monolithic coupling, where both structural and acoustic subdomains are strongly coupled and solved as a single algebraic system. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL850000.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Splitting Schemes for the Stress Formulation of the Incompressible Navier-Stokes Equations

Author(s): *Peter Minev, *University of Alberta*; Petr Vabishchevich, *Nuclear Safety Institute, Russian Academy of Sciences*.

This paper presents a novel approach to the Navier-Stokes equations which reformulates them in terms of a new tensor variable (see [1]). In the first formulation discussed in the paper this variable is proportional to the gradient of the velocity field with the pressure added to the diagonal components. In the second formulation it is identical to the stress tensor. At first glance the resulting tensorial problem is more difficult than the problem in the primitive variables. However, if combined with a proper splitting, it yields locally one dimensional schemes with attractive properties, that are very competitive to the the most widely used schemes for the formulation in primitive variables. The main advantage of such an approach becomes clear when it is applied to fluid-structure interaction problems since in such case the problems for the fluid and the structure, both written in terms of stress variables, become very similar and the stress balance boundary condition at the interface between the fluid and the structure becomes a continuity condition for the stress which is easy to satisfy in the new formulation. The only difference between the equation for the solid and the fluid phase is that the former is second order in time (hyperbolic) and the latter is first order in time (parabolic) equation. However, the same splitting schemes can be applied to both equations (see e.g. [2]) and the stability properties of the discrete problem in both domains would be the same. References: [1] Peter Minev and Petr N. Vabishchevich, Splitting schemes for the stress formulation of the incompressible Navier-Stokes equations. Submitted to: Computers&Mathematics with Applications. [2] P. Vabishchevich, Additive operator-difference schemes: splitting schemes, De Gruyter, Berlin, Boston, 2014.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: The Influence of the Ab Initio Conditions in the Numerical Solution of the Peridynamic Equation

Author(s): *David Miranda, *University of Bath, UK*.

Since peridynamic theory was developed, different numerical schemes were employed for its solution. The use of numerical methods made apparent that the choice of the ab inito conditions: initial distribution of the colocation (calculation) points and the material horizon can strongly affect the accuracy of the results. In this contribution we investigate the numerical effect of the ab inito conditions in the accuracy of the final results, development of grid effects and convergence. Benchmark examples of different scenarios were specially designed for the effect. For each example different types of ab inito conditions were employed: random distributions, lattices and lattices with perturbations. Comparisons with the Finite Element Method are provided. This paper is step toward to a set of rules for prescribing ab inito conditions, that improve accuracy and efficiency of the numerical schemes for peridynamics.

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Title: Micro-Mechanical Modeling of the Yield Behavior of Oriented Semi-Crystalline Polyethylene

Author(s): *Mohsen Mirkhalaf, Johannes van Dommelen, Leon Govaert, Marc Geers, *TU/e*.

Some polymeric materials develop a semi-crystalline micro-structure during the cooling process from the molten state. These semi-crystalline polymers are used in many different industries and in load-bearing applications. For optimal use of these materials, it is needed to predict the thermo-mechanical behaviour of these materials in a quantitative manner. During some manufacturing processes for polymeric products, such as injection molding or film blowing, the material is under shear or elongational flow resulting in an oriented micro-structure after crystallization, which leads to anisotropic mechanical behavior. The two-phase amorphous-crystalline structure is the basis of the so-called composite inclusion model, which is used and extended in this study, on hot-drawn Polyethylene tapes. The semi-crystalline material is considered as an aggregate of preferentially (due to the oriented micro-structural morphology) distributed inclusions. A hybrid interaction model is used to relate the mechanical behavior of each composite inclusion to the imposed boundary conditions of the aggregate of inclusions. Both crystalline and amorphous phases are considered to show elasto-viscoplastic behavior. In order to take into account the effect of drawing on both phases, in addition to the crystallographic oriented micro-structure, an anisotropic model is developed for the amorphous phase. A pre-stretched EGP (Eindhoven Glassy Polymer) model is incorporated into the micro-mechanical model for the amorphous phase to include an internal stress in the elastic network of the amorphous phase. Moreover, an anisotropic viscoplastic flow rule is used based on the effective stress of Hill. The yield behavior of oriented Polyethylene tapes is studied at different loading angles and the simulations are compared against the experimental results. Considerable improvements in the micro-mechanical model predictions are obtained for the yield kinetics of hot-drawn Polyethylene tapes by incorporating an anisotropic model for the amorphous phase. The results show the significance of the amorphous phase orientation on the overall yield kinetics of semi-crystalline Polyethylene.

14th U.S. National Congress on Computational Mechanics
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Title: A Heterogeneous Tissue Model for Treatment Planning in Laser Induced Thermal Therapy

Author(s): *Drew Mitchell, Christopher MacLellan, Samuel Fahrenholtz, John Hazle, Jason Stafford, David Fuentes, *MD Anderson Cancer Center*.

Introduction: Magnetic resonance-guided laser-induced thermal therapy (MRgLITT) is a minimally invasive ablative procedure, which can be used to treat primary and metastatic brain tumors, radiation necrosis, and epilepsy. Clinicians heuristically use a combination of prior information and pretreatment imaging to plan the procedural approach. While this approach is acceptable in relatively homogenous tissue environments, the laser induced heat transfer is largely unpredictable near critical structures and heat sinks, such as large vasculature and the ventricles. A physics-based model simulating heterogeneous tissue properties for a priori planning magnetic resonance-guided laser induced thermal therapy (MRgLITT) procedures in treatment of focal disease in brain is presented and evaluated. Methods: A linear superposition of analytic point source solutions to the steady state Pennes bioheat transfer equation simulates laser-induced heating in brain tissue. An approximation to the source term allows computation of heterogeneous tissue properties. Optimization of tissue-dependent optical attenuation coefficients by an interior point method trains models with 1,2,4,8, and 16 tissue labels. In N=30 MR thermometry datasets, modeling prediction accuracy is quantitatively determined by the Dice similarity coefficient (DSC) between model-predicted and measured ablation regions (T>57 degrees C). Results: Median DSC values for homogeneous and heterogeneous tissue models were approximately 0.86, independent of number of tissue labels, as expected for lesions already modeled well by a homogeneous model. The cases in the bottom quartile, where the homogeneous model failed, spanned DSC values from 0.68 to 0.79 for a single tissue label and improved to a range from 0.76 to 0.82 when modeled with 8 tissue labels, indicating a significant improvement in the ability of this model to capture heterogeneities responsible for underperformance in predictive capability of homogeneous models. Conclusion: This work accomplishes more accurate treatment outcome prediction by modeling up to 16 different tissue types with independent optical properties and represents another step toward commercialized MRgLITT treatment planning programs capable of improving pre-treatment planning and treatment quality. Future work will include more capable segmentation methods, such as random forest, and modeling with additional relevant physical parameters, and prediction from a transient solution of the Pennes bioheat equation.

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Title: Dynamic Rupture Simulation of a Tunnel Subjected to Fault Displacements Using Parallel 3D-FEM

Author(s): *Yuta Mitsuhashi, Fujio Uchiyama, *KOZO KEIKAKU ENGINEERING Inc.*; Gaku Hashimoto, Hiroshi Okuda, *The University of Tokyo*.

In recent years, numerical simulations of fault displacements have become crucial for evaluating the soundness of underground structures during an earthquake. Fault displacement is defined as the relative movement present on either side of a fault plane and occurs as the result of the rupture of the earthquake source faults. Previous studies have been conducted using the finite difference method, the finite element method, etc. A few samples of the damage in tunnels subjected to fault displacements have been found in Japan, such as Shioyaganigawa drainage tunnel at the Great Hanshin Earthquake, 1994 and Tanna tunnel at the Kita-Izu Earthquake, 1930. It is not easy to avoid the fault in the case of both bridge and tunnel because of its linear shape. Reduction of the effect of the fault displacements is possible by implementing large span girder in the case of bridge but not for the case of tunnel. We also note that there are still many unknown issues such as the mechanism of the damage, the effect of the thickness of the fault, etc. In the previous studies, an underground structure and surrounding soil is modeled by solid elements or spring elements, because of the contrast of the size between the fault and the structure, and a limitation of FEM storage. The tunnel subjected to the fault displacements is the coupled problem of the soil and the structure. We should consider the large memory requirement when we model both the structure and a part of soil. In addition, we should keep in mind that the dynamic effect could not be considered when the static displacements boundary condition is applied onto the surface of the model. In our study, we consider the underground structure, the soil and the entire fault crossing the structure in a FE model. A large-scale parallel 3D-FEM is performed in such a way that the spontaneous rupture process of a fault is reproduced. This research was conducted using the finite element method code FrontISTR, which can perform parallel computation of large-scale models. We evaluate the effect of soil properties and fault model to the response of structure. We show that soft soil reduce the response stain of structure, modeling strong motion generation area effect the response of structure and response strain is increase little by considering the dynamic effect.

14th U.S. National Congress on Computational Mechanics
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Title: Analysis of Free-Surface Flow Interacting with an Elastic Beam Using Mesh-free Particle Method and Finite Element Method

Author(s): *Naoto Mitsume, Tomonori Yamada, Shinobu Yoshimura, *The University of Tokyo*.

Interactions between waves and structures are often important for safe and optimal design of facility located along coastal line. To analyze these fluid–structure interaction (FSI) phenomena involving free-surfaces, we have been developing an FSI model [1] combining mesh-free particle method and finite element method. This model has advantages in dealing with moving boundaries in the free-surface flow computation and having high-reliability in the structural computation. By adopting a polygon wall boundary model [2], which enables us to use triangular polygons as wall boundaries in the free-surface flow analysis, fluid–structure interfaces in both the fluid and structural computations are geometrically identical in our proposed model. We have conducted verification tests as compared to numerical results obtained by other FSI models. In this study, we conduct a validation test for the proposed model by simulating an experiment of free-surface flow interacting with an elastic beam [3]. We perform numerical simulations by changing time spacing values, coupling schemes, and spatial resolutions, and discuss these effects. REFERENCES [1] Mitsume, N., Yoshimura, S. and Yamada, T. Consistent Interface Fluid-Structure Interaction Model based on Mesh-free Particle Method and Finite Element Method, 12th World Congress on Computational Mechanics, Seoul, Korea, (2016). [2] Mitsume, N., Yoshimura, S., Murotani, K. and Yamada, T. Explicitly Represented Polygon Wall Boundary Model for the Explicit MPS Method. Computational Particle Mechanics, Vol. 2, No. 1, pp. 73–89, (2015). [3] SPHERIC BENCHMARKS. http://canal.etsin.upm.es/ftp/SPHERIC_ BENCHMARKS/

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Balancing Domain Decomposition Method for Finite Element Analysis of Large-Scale Assembly Structure Modeled Using Millions of Multi-Point Constraints

Author(s): *Tomoshi Miyamura, *Nihon University*.

The present author [1] proposed a method to incorporate multi-point constraints (MPCs) into the balancing domain decomposition (BDD) method [2], which is a preconditioner for the conjugate gradient (CG) method. The preconditioner of the BDD method consists of the Neumann-Neumann preconditioner and the coarse grid correction. In this study, the method is improved and applied to an analysis of a large-scale assembly structure of complex geometry. Each component of a structure is modeled as a fine mesh of solid elements. The meshes of components are assembled using MPCs. Time for generating a finite element mesh can be reduced drastically by generating meshes of components independently and by assembling those meshes using MPCs. In the present method, MPCs are formulated using the Lagrange multiplier and incorporated into the BDD method using the preconditioned conjugate projected gradient (PCPG) method. The constraints are also introduced in the coarse grid problem using a penalty method. A set of MPCs is decomposed into a number of independent groups of MPCs, and the projections in the PCPG method for the groups are conducted in parallel. A combined MPI and OpenMP programming model is adopted for parallel implementation of the BDD method using the framework of ADVENTURE system [3]. Computation cost to consider MPCs is not expensive and convergence property of the BDD method is not affected by the incorporation of the MPCs. As an illustrative example, a mesh of a super-high-rise building with ground is generated as an assembly of component meshes connected using MPCs. Each component mesh is made of hexahedral elements. The number of elements is 28,363,862, that of nodes is 37,311,413 (111,934,239 DOFs), and that of MPCs is 2,962,659. The seismic response analysis of the building is conducted using K computer. It is demonstrated that the present method enables a structural analysis using an assembly model of a structure of complex geometry in which millions of MPCs are included. References: [1] Miyamura, T., Incorporation of multipoint constraints into the balancing domain decomposition method and its parallel implementation. Int. J. Numer. Methods Eng., 69, 326-346, 2007. [2] Mandel, J., Balancing domain decomposition, Commun. Numer. Methods Eng., 9, 233-241, 1993. [3] Home page of ADVENTURE Project, http://adventure.sys.t.u-tokyo.ac.jp/

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Non-Local Formulation for Transport and Damage in Porous Media

Author(s): *Mostafa Mobasher, Luc Berger-vergiat, Haim Waisman, *Columbia University*.

We present a novel damage-poroelastic model for analyzing the failure response of porous media in geomechanics applications. In this new approach, a gradient non-local permeability that leads to non-local transport and consequently non local damage, is introduced. Damage evolution is function of an equivalent strain measure that is computed from non-local permeability using an inverse permeability-strain constitutive relation. A monolithic, mixed finite element method is proposed to solve the coupled system with a displacement-pressure-regularized permeability (u-p-\tilde{\kappa}) element formulation. The system is linearized and solved using Newton's method and an implicit Newmark scheme is used to evolve the system in time. A consistent Jacobian matrix and residual vector are derived analytically and a bilinear damage model is used to evolve the damage. Numerical examples considering hydraulic fracture problems in 1-d and 2-d and damage enhanced consolidation are presented and discussed. The proposed non-local model results are compared with local damage-permeability models. While the local models are shown to suffer from mesh dependence and non-physical spurious oscillations in strain, permeability and fluid pressure evolution, the proposed model is reliable and seems to overcome all these limitations.

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Title: The Thick Level Set Model for Fracture: A Theory Allowing the Coupling of Cohesive and Diffuse Approaches to Fracture

Author(s): *Nicolas MOES, Benoit Le, Gregory Legrain, *Ecole Centrale de Nantes*.

The Thick Level Set Model for fracture is based on a regularization of local damage models through an eikonal inequality. As damage proceeds, a crack is introduced in the model allowing for displacement discontinuity. In previous use of the TLS approach, the crack was introduced when the material was fully damaged (and was thus a traction-free crack). In this paper, we consider the possibility to introduce a cohesive crack prior to the material being fully damaged. The obtained TLS model is able to drive simultaneously both the diffuse and cohesive zone of the model. The advantages of this coupled modeling will be described.

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14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Modified Non-Local GTN Damage Model for High Strain Rate Loading

Author(s): *Nisha Mohan, Gary Dilts, *Los Alamos National Lab*.

With local continuum damage models, the results are inherently highly sensitive with respect to the spatial discretization length. Therefore to overcome mesh dependence, a modified non-local formulation of GTN damage model is proposed here, to work under an Eulerian explicit finite volume framework. The GTN model also takes advantage of the equations of states to evolve the material properties under high pressures and temperatures. The model is applied to simulate the fracture mechanical test of a typical metallic pressure vessel. It captures the salient features of damage propagation, such as porosity led shear band-like structures and fragmentation under ductile failure. Hence, it is seen to capture damage realistically compared with experimental results. Post-processing is based on the porosity and stress state development at various stages of crack initiation and propagation.

14th U.S. National Congress on Computational Mechanics
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Title: Arbitrary Polygonal Elements Using Discontinuous Petrov Galerkin (DPG) Method

Author(s): Ali Vaziri Astaneh, *Jaime Mora Paz, Federico Fuentes, Leszek Demkowicz, *University of Texas at Austin*.

Developing finite elements with unconventional shapes has gained a significant interest over the past decade. In this work we present the first endeavor to construct arbitrary polygonal elements using the Discontinuous Petrov Galerkin (DPG) methodology. For simplicity we consider the two-dimensional Poisson's equation as the model problem. The DPG method is known to be well posed for several variational formulations [1]. We choose the ultraweak formulation (simultaneously relaxed first-order equations) due to implementation advantages for non-traditional elements. In this formulation, both scalar and vector (flux) field variables lie in the L2 energy space, as such no conformity across the element interfaces needs to be satisfied. The trial basis functions for the polygonal element are obtained by restricting the basis functions of a triangular/quadrilateral element containing the domain of each polygonal element. Even though the test functions are in H1 and H(div) energy spaces, the same strategy is applied since a central component of DPG is to use broken test spaces, i.e. the support of the test functions is a single element. The system of equations resulting from the DPG method only contains the discretized trace variables on the mesh skeleton playing the role of Lagrange multipliers. A conforming discretization of the trace variables is carried out by using one-dimensional H1 and L2 shape functions along the element edges. We present various numerical examples using arbitrary polygonal meshes and demonstrate the delivery of optimal convergence rates (for the field variables) in the L2 norm. We also investigate the performance of the presented approach for regular grids being cut by arbitrary lines representing the faulting phenomenon that exists in heterogeneous crustal structures. Extension of the presented technique to arbitrary three-dimensional polyhedral elements is in progress. [1] Carstensen, Carsten, Leszek Demkowicz, and Jay Gopalakrishnan. "Breaking spaces and forms for the DPG method and applications including Maxwell equations." Computers & Mathematics with Applications 72.3 (2016): 494-522.

14th U.S. National Congress on Computational Mechanics
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Title: A Coarse-Grained Brownian Molecular Dynamics Model of von Willebrand Factor Multiscale Response to Flow

Author(s): *Michael Morabito, Wei Wei, Chuqiao Dong, Alparslan Oztekin, Edmund Webb III, Xuanhong Cheng, Xiaohui Zhang, *Lehigh University*.

In healthy bodies, the formation of blood clots stops bleeding due to vascular damage, and the plasma protein von Willebrand Factor (vWF) plays an indispensable role in blood clot formation. vWF remarkably senses increased hydrodynamic forces at the site of vascular damage and responds by undergoing a conformational change to unmask sites for bioreactivity. However, unfolding on two different length scales must be considered in order to understand vWF's role in physiological processes. Macromolecular unravelling is the first unfolding mechanism of vWF and facilitates blood clotting by revealing binding sites for platelet receptors. The second unfolding response occurs on the intra-monomer level where the A2 domain of vWF unfolds under sufficient hydrodynamic force thereby revealing cleavage sites that permit vWF scission. The basic biological role of vWF in blood clotting is relatively well known; however, underlying biomechanical mechanisms motivating these physiological phenomena are poorly understood and desirable for applications in targeted drug delivery and disease treatment. We introduce a new coarse-grained molecular dynamics model that more accurately describes the architecture inherent to vWF by considering both length scales. This model is parameterized by the single-molecule pulling experiments conducted by Zhang et al [1]; therefore, the obtained simulation statistics are physiologically germane. We employ a bead-spring description of vWF and perform Brownian Molecular Dynamics Simulations (BMDS) derived from the Langevin equation. We initialize a vWF multimer in an elongational flow field and study the dynamical response occurring on both length scales such as radius of gyration and the distribution of internal tensile force in circulating multimers, respectively. This model is capable of capturing the internal dynamics of the A2 domain in the vWF monomer, which is crucial for understanding vWF response to flow [1]. We examine the likelihood and most probable location of vWF proteolysis by the metalloprotease ADAMTS13 through examination of A2 domain unfolding. Further, we offer explanation to the existence of discrete size distributions of vWF in vivo, rather than a continuous size distribution, in light of these BMDS results. We examine flow fields and multimers of varying strength and length, respectively, as well as identify some of the hurdles associated with simulation of long polymer chains and internal polymer dynamics. Lastly, this work identifies the importance of properly implementing stochastic Brownian motion and hydrodynamic interactions, and addresses length-scale dependent simulation convergence. [1] X. Zhang, Science. 324, 1330 (2009).

14th U.S. National Congress on Computational Mechanics
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Title: Model Order Reduction of Dynamic Skeletal Muscle Models

Author(s): *Mylena Mordhorst, Oliver Röhrle, *University of Stuttgart*.

Forward simulations of three-dimensional continuum-mechanical skeletal muscle models are a complex and computationally expensive problem. Considering a fully dynamic modelling framework based on the theory of finite elasticity is expensive and challenging as the muscles' mechanical behaviour requires to consider a highly nonlinear, viscoelastic and incompressible material behaviour. The governing equations – the momentum balance subject to an incompressibility constraint and a nonlinear constitutive equation – yield a parametric, nonlinear second-order differential algebraic equation (DAE), which has similar properties as systems resulting from fluid dynamics problems. Especially because of their additional constraint equation and strong nonlinearities, these systems represent a challenge to model order reduction techniques. To decrease the computational effort of solving the resulting system, we apply projection-based model order reduction techniques. Here, we obtain the reduced basis by means of a proper orthogonal decomposition (POD). In detail, we perform a Galerkin block-projection, where we use different projection spaces for the displacement, velocity and pressure degrees of freedom. This approach turned out to be the best to maintain the stability of the system. Furthermore, the online evaluation of the projected nonlinear operator can be addressed by different methods. In this contribution, we want to show a comparison of the effectiveness of applying the discrete empirical interpolation method (DEIM) and the energy conserving sampling and weighting (ECSW) hyper reduction method.

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Title: Improvement of Near Wall Velocity Prediction Using Mask in a Penalised Vortex-In-Cell Algorithm

Author(s): *Francois Morency, *ÉTS*; Héloïse Beaugendre, *Bordeaux-INP, IMB, Inria Cardamom*.

Immersed boundary methods (IBM) are attractive to compute the trajectory of a solid body in a fluid in motion. When the solid to the fluid density ratio is large, aerodynamic forces and gravity mostly drive the body motion. IBM allows for easily tracking the body using level set functions and a Cartesian mesh, avoiding the need of remeshing around the body surface. The main drawback of IBM is the blurring of the wall position, reducing the numerical order of the method near the wall. This especially reduces the accuracy of the shear stress prediction at the wall. The objective of this presentation is to suggest a mask function that improves the quality of the velocity field prediction near the wall. The mask is formulated for a penalized VIC algorithm. The first sub-objective is to build a mask function based on a velocity profile derived from the boundary layer equations. As the VIC formulation solve the vorticity equations, the mask should return the vorticity for a given wall normal distance. The second sub-objective is the quantification of the mask effects on the boundary layer velocity field around a streamlined body, such as an immersed flat plate. In particular, flow field will be computed around various positions and orientation of the flat plate such that the grid nodes do not coincide with solid-fluid interface. The third sub-objective is the verification of the mask effect on flow prediction around a bluff body, such as cylinders. The vorticity form of the Navier-Stokes equations is solved with a Vortex-In-Cell (VIC) algorithm [1]. The penalization method [2] enforces the no-slip boundary condition on the solid wall boundaries. Level set functions are used to capture interfaces and compute rigid motions of the solid bodies. The level set function is the distance to the solid-fluid interface, with a negative value inside the solid. At solid-fluid boundaries, a mask is used to distribute the wall effect on adjacent nodes[3]. The proposed mask take into account some of the physic of the near wall flow compared to the commonly used Dirac function. References: [1] Mimeau, C., et al., Vortex penalization method for bluff body flows. International Journal for Numerical Methods in Fluids, 2015. 79(2): p. 55-83. [2] Angot, P., C. Bruneau, and P. Fabrie, A penalization method to take into account obstacles in incompressible viscous flows. Numerische Mathematik, 1999. 81(4): p. 497--520. [3] Beaugendre, H., et al. Computation of Ice Shedding Trajectories Using Cartesian Grids, Penalization, and Level Sets. Modelling and Simulation in Engineering, 2011. 2011

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Title: Monolithic Linear Equation Solver for Parallel Finite Element Method

Author(s): *Naoki Morita, Gaku Hashimoto, Hiroshi Okuda, *The University of Tokyo*.

Finite element analysis based on domain decomposition method is widely used in science and engineering field. Along with the development of computers and the necessity of highly accurate analysis, the scale of numerical analysis is increasing. As a numerical method for solving large-scale linear equations, we focus on the SPIKE method from the viewpoint of being suitable for parallel execution on the many core environment [1, 2]. In many cases dealing with large-scale problems, the decomposed domain for parallel computation is determined under a condition for reducing interregional communications. Generally, such decomposed domains do not form a block band matrix because a decomposed domain has a relationship with a plurality of decomposed domains. However, the conventional SPIKE method is applicable only to a band matrix as a coefficient matrix. In order to apply to the linear equations obtained from the finite element method, there are restrictions such as necessity of an appropriate reordering of node numbers and performing domain decomposition to obtain a band matrix. Because of these restrictions, the condition of reducing interregional communications in not satisfied. In this research, we propose a method to extend the SPIKE method based on information of overlapping domain decomposition for solving these restrictions. Since each decomposed domain holds the communication information with other domains, computation of SPIKE method can be performed under the condition for reducing interregional communications. Further, iterative methods are employed as a local solver for solving the inside of the decomposed domain and as a solver for solving the global problem. The proposed method is used as preconditioning for iterative method and its performance is evaluated by numerical examples. [1] E. Polizzi and A. H. Sameh, A parallel hybrid banded system solver: the SPIKE algorithm, Parallel Computing, Elsevier, Vol. 32, pp. 177-194 (2006). [2] K. Mendiratta and E. Polizzi, A threaded SPIKE algorithm for solving general banded systems, Parallel computing, Elsevier, Vol. 37, pp. 733-741 (2011).

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Title: Adaptive Meshing Strategy Based on Topo-Metric Data for the Dam Break Inundation Assessments

Author(s): *Mahdi Moslemi, *Ecole de technologies Supérieu*; Azzeddine Soulaimani, *Ecole de technologies Supérieure*; Georges W.Tchamen, *Hydro-Quebec*.

Flood maps are the final product of the dam failure studies required by the dam safety regulations. The flood limit which represents the maximum envelope reached by the flood wave is generally the result of a dam break scenario simulated by a hydraulic numerical model. However, a numerical model uses only a limited portion of the bathymetry data available to build the terrain model (2D mesh plus topo-metric elevation at nodes). Particularly in cases where the topo-metric data has been recorded by the Lidar, this data is estimated in several million of points. But, the hydraulic numerical models rarely exceed hundreds of thousands of nodes, in particular due to the computer constraints and time associated with the operation of these models. The production of the final flood map requires consistency between projected levels and elevations for all points on the map. This verification may be tedious if the area is large and there are several small secondary valleys of tributary streams which have not been represented by the original hydraulic numerical model. The aim of this work is to propose an automatic strategy of remeshing which uses the envelope of the maximum dimensions reached by the original model coupled with the available Lidar data to produce an improved mesh that will succeed in capturing accurately the wet/dry fronts and the overflows of the secondary valleys. The algorithm is based in few basic steps such as: (i) find the elements cut by the envelope of the wet/dry interfaces, (ii) project the topo-metric points onto the cut elements, (iii) if these points are very close to the interface or if they are found in a valley or if they are more elevated than the corresponding cut elements then these points will be added to the previous nodes which be included in a subsequent triangulation step, and (iv) re-run the simulation on the new mesh. This algorithm has been implemented and validated in the study of a dam break flow on a complex river bathymetry.

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Title: Simulation of Fracture, Fragmentation, and Debris Field Formation in Glass Lites Under Blast Loading using the Applied Element Method

Author(s): *Jonathan Moss, Adam Howe, Matthew Whelan, David Weggel, *UNC Charlotte*.

The Applied Element Method (Meguro and Tagel-Din, 2000), a variant of the rigid body spring model (Kawai, 1978), is a computational alternative to the Finite Element Method that offers distinct advantages for the simulation of problems with extensive fracture and fragmentation. These capabilities render this methodology particularly attractive within the subset of blast and impact problems, where the prediction of the damaged state of the structural system is usually of greatest importance. Post-blast structural forensic investigation, aided by collection of high-resolution 3D scanning and advanced numerical simulation, is one particular area where such capabilities are necessary for hypothesis testing. In this study, the Applied Element Method is implemented as a physics engine for the prediction of glass fracture, fragmentation, and debris field formation following explosive events to aid in post-blast structural forensic investigations. This presentation will provide a brief introduction to the Applied Element Method with emphasis on the nonlinear geometry and nonlinear constitutive implementations required to develop a model of a glass lite conventionally supported by aluminum window mullions. Dynamic verification of the model using measured modal parameters obtained through experimental modal analysis will be discussed, followed by validation of the predictive fidelity in the linear and nonlinear regimes through comparisons with experimental data. These comparisons include static load testing of a glass lite supported in an aluminum window mullion and subjected to uniform loading through the initiation of fracture. Load and point displacement measurements as well as full-field 3D scans obtained during the test program are used to assess the model correlation with the glass deformation and fracture pattern. Following this static validation, the simulations are extended to dynamic analysis of glass lites subjected to blast loading from satchel-sized charges with short stand-off. Comparisons are developed with experimental data obtained from extensive open-arena blast testing of facade walls, each containing six glass lites, to assess the potential of the Applied Element Method to serve as a computational platform for post-blast forensic investigation. Kawai, T. (1978) “New discrete models and their application to seismic response analysis of structures,” Nuclear Engineering and Design, 48(1), 207-229. Meguro, K. and Tagel-Din, H. (2000) “Applied Element Method for structural analysis: theory and applications for linear material,” Structural Engineering/Earthquake Engineering JSCE, 17(1). 21-35.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: The Schwarz Alternating Method in Solid Mechanics

Author(s): *Alejandro Mota, Irina Tezaur, Coleman Alleman, *Sandia National Laboratories*.

We advance the Schwarz alternating method as a means for concurrent multiscale coupling in finite deformation solid mechanics. We prove that the Schwarz alternating method converges to the solution of the problem on the entire domain and that the convergence rate is geometric provided that each of the subdomain problems is well-posed, i.e. their corresponding energy density functions are quasi-convex. It is shown that the use of a Newton-type method for the solution of the resultant non- linear system leads to two kinds of block linearized systems, depending on the treatment of the Dirichlet boundary conditions. The first kind is a symmetric block-diagonal linear system in which each diagonal block is the tangent stiffness of each subdomain, i.e. the off-diagonal blocks are all zero and the coupling terms appear only on the right-hand side. The second kind is a nonsymmetric block system with off-diagonal coupling terms. Several variants of the Schwarz alternating method are proposed for the first kind of linear system, including one in which the Schwarz alternating iterations and the Newton iterations are combined into a single scheme. This version of the method is particularly attractive, as it lends itself to a minimally intrusive implementation into existing finite element codes. Finally, we demonstrate the performance of the proposed variants of the Schwarz alternating method on several one-dimensional and three-dimensional examples. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Discrete Particle Techniques For Multiscale Modeling Of Fragmentation Of Blood Clots

Author(s): *Debanjan Mukherjee, Shawn C. Shadden, *Univ. of California, Berkeley*.

Fragmentation of a blood clot, often referred to as embolization, releases freely floating clot debris (emboli) into the bloodstream. These emboli can travel to critical vascular beds, and impede blood supply to vital organs including the brain and the kidneys. In particular, embolic occlusions in the brain comprise a prominent cause of stroke, leading to death and disability worldwide. This motivates the need for developing a comprehensive understanding of clot embolization. However, the underlying biomechanical behavior of a blood clot is governed by complex multiscale phenomena, with a strong connection to hemodynamic loading induced by pulsatile blood flow within arteries. In addition, a realistic, patient-specific clot possesses arbitrary shape, morphology, and heterogeneous microstructure, which need to be accounted for. These factors render significant challenges towards developing a biomechanical model for embolization. Addressing these factors, especially in the context of resolving an essentially discrete and discontinuous phenomenon like fragmentation, is often difficult using existing continuum mesh/grid based techniques. In this work, we present an innovative, discrete particle based multi-scale computational model for clot embolization. Blood clots are modeled as mesoscopic aggregates of discrete, computational, off-grid particles/elements, and embolization biomechanics is recovered via inter-particle interactions governed by effective forces and potentials. Coupling with background hemodynamics is achieved using a two-way coupled fictitious domain finite element method. The overall framework is illustrated using a model system comprising a clot embedded within an idealized channel with width equivalent to that of the human common carotid artery, and a measured pulsatile flow profile at the channel inlet to drive the flow. A variety of clot geometries, both idealized as well as experimentally obtained, are used for this model. Through numerical experiments using this model system, we demonstrate the capability of the proposed methodology to capture embolization, starting from initiation of fragmentation up until the formation of a completely dissociated embolus. Acknowledgement: This research was supported by the American Heart Association award no: 16POST27500023.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Communication-Free Mesh Multiplication Using Pairing Function

Author(s): *Renato N. Elias, Alvaro L. G. A. Coutinho, *PEC/COPPE/UFRJ*; Jose J. Camata, *NACAD/COPPE/UFRJ*.

Computational power has been growing in the last decades and we now can run simulations on unstructured meshes with billion of elements. However, building such large meshes is still a cumbersome task even for parallel computers. Adaptive mesh refinement algorithms for distributed meshes usually rely in peer-to-peer message exchanges among processes to keep nodes and elements creation (or destruction) consistent, thus, increasing computational costs. A different approach for building large-scale parallel meshes is based on uniform element subdivision, a technique usually called mesh multiplication. In this method, each element of the original coarse mesh is subdivided into smaller elements following a common pattern for the entire mesh. By applying the same subdivision to all tetrahedra in the mesh, a new and finer mesh, 8 times larger and more refined is created. The process can be applied hierarchically creating different refinement levels. The benefit of such approach against traditional adaptive mesh refinement is that element creation is known a priori and follows a constant pattern. Thus, distributed parallel processes may apply the same algorithm independently and communication costs decreases substantially. In this work, we propose a fast tetrahedra mesh multiplication technique developed for EdgeCFD code. EdgeCFD employs edge based data structures to speedup computations, save memory and reduce indirect memory address operations. It also employs a local numbering scheme so as mesh partitions may grow independently. For distributed memory parallelism, EdgeCFD relies on non-blocking peer-to-peer message exchanges based on a master-slave relationship but it also may run in shared memory platforms as entities are blocked to avoid memory dependency in major loops. The mesh multiplication method proposed here employs pairing functions to compute new global indexes independently from a pair of node of the coarser mesh by each parallel processor. Therefore, no communication is required to keep the parallel interface among processes consistent. A large scale test-problem is presented to demonstrate the efficiency of the method.

14th U.S. National Congress on Computational Mechanics
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Title: A Combined Phase Field and Crystal Plasticity Approach for Capturing Thermo-Mechanical Behavior of Polycrystalline Rock Salt

Author(s): *SeonHong Na, WaiChing Sun, *Columbia University*.

Rock salt or halite is one of the major materials used for nuclear waste disposal. The desired characteristics of rock salt, i.e. the high thermal conductivity, low permeability and self-healing are highly related to the crystalline microstructure. Conventionally, this microstructural effect is often incorporated phenomenologically in macroscopic models. Nevertheless, effort to directly simulate the interplays among micro-mechanical mechanisms, such as micro-cracking, inelastic dilatancy, grain boundary sliding and dislocation creeping, which may bring more reliable and robust forward predictions for the long-term thermo-mechanical behavior of salt, are lacking. The goal of this research is to fulfill this knowledge gap. In particular, we first formulate a computational framework that may predict multi-slip system crystal plasticity of single crystal in rate-independent and rate-dependent regimes. Using this as a starting point, we introduce an anisotropic phase-field based model in which displacement and temperature jumps are regularized to model the grain boundary where the temperature-dependent plastic flow is parallel to the ground boundaries. The texture of the polycrystalline salt is assumed to be random by assigning different sets of orientations to each grain. The grain boundary is approximated using the crystal plasticity constitutive model with single slip system to include the inelastic behavior, while the fracture response is captured via the evolving phase field. Numerical examples demonstrate that the proposed model is able to capture the brittle-ductile transition under various of loading rate, temperature and confining pressure with a minimal set of material parameters.

14th U.S. National Congress on Computational Mechanics
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Title: Multiphysics Life Prediction Damage Model of a Turbine Engine Blade Disk Attachment

Author(s): *Samir Naboulsi, *HPCMP PETTT CSM Lead - AFRL DS*.

Life prediction of turbine engines is crucial part of the management and sustainment plan to aircraft jet engine. Recently the failure of engines on four jet aircraft overseas during the past few years has prompted the National Transportation Safety Board (NTSB) to issue an "urgent" recommendation to increase inspections of the engines on U.S. aircraft. At issue are older engines found on a small number of jets. The Federal Aviation Administration (FAA) issued a rule in March 2010 requiring inspections of the engines within 50 flights, and repeat inspections every 175 flights thereafter. The disk-blade damage is complex multi-physics phenomena. It is mainly driven by contact mechanics, high speed aero-flow, high temperature, vibratory motion, and environment degradations. Fretting is one of the primary phenomena that leads to damage or failure of blade-disk attachments. Fretting is a complex phenomenon that depends on geometry, loading conditions, residual stresses, and surface roughness, among other factors. The objective of the present investigation is to introduce physic based modeling to understand damage mechanism in an actual blade-disk attachment. Its intent is to better understand damage in realistic scenario providing designer better understanding of the mechanism itself without addressing design issues. Simulating damage in blade-disk is an ongoing effort. Earlier works modeled fretting fatigue damage using a unique energy based contact mechanics approach. The model has been evolving in the past few years, and it has been addressing various fretting conditions. The influence of a microstructure length scale was studied by implementing crystal plasticity model to address some of the limitation of traditional macroscopic plasticity models. Further, under pre-assumed conditions, the effects of thermal diffusion and temperature fluctuation during engine operation modeled. The coupled thermos-mechanical simulation with unified viscoplasticity Bodner-Patom model and fatigue contact damage captured couple of material damages in addition to fretting. First, the lower section of the blade where the stresses are most significant exhibited higher damage. Second, thermal damage found to be most significant at the mid-section of the blade airfoil leading edge. Based on these results, the present effort focused on further enhancing the damage prediction. A new thermal fatigue law based on Lemaitre developed with temperature dependent material properties. Further, a couple mechanical-diffusion formulation implemented to capture the oxygen ingress and eventually model the oxidization/embrittlement. Finally, numerical simulations will be presented.

14th U.S. National Congress on Computational Mechanics
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Title: Full-Eulerian XFEM for Fluid-Structure Interaction Analysis

Author(s): *Toshiki Nagai, Kurt Maute, *U. Colorado*.

Fluid-structure interaction (FSI) analysis is generally performed using an Arbitrary Lagrangian-Eulerian framework (ALE-FSI). The coupling of the solid and fluid phases is based on a Lagrangian interface description. The fluid domain is discretized by a body-fitted mesh that follows the structural deformations along the fluid-solid interface. ALE-FSI is widely used due to its ability to accurately represent the interface geometry. However, the need for body-fitted fluid meshes impose severe limitations on the level of structural deformations. This includes in particular topological changes, such as structural contact phenomena. Large structural deformations and contact play an important role for a wide range of applications, e.g. tires on a wet surface. To numerically simulate such problems, we present a computational framework where both the structural and the fluid response are described by an Eulerian approach. The fluid-solid interface is captured by the Level set method (LSM). The weak form of the governing equations in the fluid and solid domains are discretized by a Heaviside-enriched extended finite element method (XFEM), defined on a fixed background mesh. Through numerical experiments we study the convergence behavior and stability of the proposed framework for 2D FSI problems where the structure undergoes large deformation and contact and the flow is incompressible and laminar.

14th U.S. National Congress on Computational Mechanics
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Title: Development of a Three-Dimensional Crack Analysis System Using XFEM and Evaluation of Its Accuracy

Author(s): *Toshio Nagashima, *Sophia University*.

A three-dimensional crack analysis system based on the eXtended FEM (XFEM) using hexahedral elements has been developed. The system requires finite element data without considering the crack geometry and three-dimensional crack surface data explicitly defined by a set of triangular patches. Two kinds of signed distance functions are employed to model the crack implicitly. Enrichment nodes are automatically determined in the system and then a hexahedral crack tip element is partitioned into several pentahedrons and integrated. Two kinds of in-house XFEM codes are utilized in the developed system. One uses a crack tip element enriched with both the asymptotic bases and the Heaviside function, and another uses only the Heaviside function. J-integral at a crack front is evaluated by the domain integral method and crack geometry is updated by a crack propagation law when crack propagation is considered. The system is verified through solving several stationary and propagation crack problems.

14th U.S. National Congress on Computational Mechanics
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Title: Source Transformation Algorithmic Differentiation of Memory Allocation and Pointer Manipulation

Author(s): Laurent Hascoet, *INRIA Sophia Antipolis*; Jean Utke, *Allstate*; *Sri Hari Krishna Narayanna, *Argonne National Laboratory*.

Proper handling of pointers and the (de)allocation of dynamic memory in the context of an adjoint computation via source transformation algorithmic differentiation has so far had no established solution that is both comprehensive and efficient. Therefore, such tools have required the input code to be rewritten to exclude all memory allocation and pointer manipulation. For many input codes, this is an unacceptable requirement. We have implemented a memory management library called ADMM to support the use of dynamic memory allocation within codes being differentiated. We will shown how this library can be used to differentiate the multibody code in the adjoint mode.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Numerical Modeling of Tornado-Like Vortex and Its Interaction with Low-Rise Building

Author(s): *Zoheb Nasir, *Post-Doctoral fellow*.

A numerical model depicting the WindEEE Dome tornado simulator and a simplified generic numerical model representing the same simulator are used to simulate tornadoes over a bluff-body, which represents a low-rise building. Several geometric simplifications are made over the complex numerical model to obtain the simplified version using proper boundary conditions. This simplification process once verified in the present study can be used to obtain simplified numerical models for complex laboratory tornado simulators irrespective of their geometrical shape and size. For verification purpose, external pressure coefficients along the surfaces of the bluff-body for both complex and simplified numerical models are compared with results obtained from the experimental model. In order to enhance the verification process, although the tornado is kept stationary, two different locations of tornado center are considered. For location 1, center of tornado coincides with the center of the bluff-body, while for the other location (location 2), tornado is placed so that the center of the bluff-body coincides with the core radius (location of maximum tangential velocity of a tornado-like vortex) Preliminary study shows that, for location 2, pressure distribution is quite identical between both numerical models and experimental models. However, the numerical models predict slightly higher suction compared to the experimental model. Further, suction occurs along all the surfaces of the bluff-body, which indicates ground suction field due to the angular momentum of the tornadic flow dictates the overall pressure distribution rather than the bluff body – tornado interaction at core center.

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Title: Establishing the Mechanical Properties of Pelvic Floor Muscle by Using MRI and an Inverse Method

Author(s): *Renato Natal Jorge, *INEGI, Faculty of Engineering,*; Elisabete Silva, Sofia Brandão, Marco Parente, *INEGI, Faculty of Engineering, University of Porto, Porto, Portugal*; Teresa Mascarenhas, *FMUP*.

The biomechanical assessment of the pelvic floor (PF) tissues is important to understand the pelvic disorders and also to improve clinical outcomes, as well as the decreased elasticity of the tissues often causes inability to maintain the normal positions of the pelvic organs. These disorders may result from inadequate biomechanical properties of the supportive structures such as muscles, ligaments or pelvic fascia. By using MRI information and an inverse method based on the finite element method a procedure is presented in the present work. Distinct values of the elasticity of the pelvic floor muscles (PFM) from women with pathological disorders and also from asymptomatic women are present. To determine the biomechanical properties of the PFM with incontinence and prolapse, and without pathologies was used a non-invasive methodology through of computational models coupled with information acquired by Magnetic Resonance Imaging (MRI). The estimation of the in vivo biomechanical properties evidenced a significant difference between the different groups of women. When comparing the incontinent women with prolapsed women, significant difference in the properties was obtained. The results showed that the PFM of incontinent women have an elasticity 38% lower than women without pathology and there were no morphological differences between the two groups, while for the women with prolapse was 43% higher. The computational models can represent a promising possibility to determine the in vivo biomechanical properties of the PFM, leading to a relationship between for the incontinent women and women with prolapse.

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Title: Modeling and Simulation of the Mechanical Behavior of Fiber Networks with Cohesion

Author(s): *Vineet Negi, Catalin Picu, *Rensselaer Polytechnic Inst.* .

Fiber networks are a common occurrence in artificial and biological materials. Rubber, epoxy and gels are molecular networks, connective tissue is a network of collagen and elastin fibers, while various types of polymeric fibers are used for consumer products ranging from baby diapers to non-woven protective clothing. In many of these systems, the fibers interact cohesively and are thin enough for cohesion to play effectively against the bending resistance and have an important role in mechanics. In this work, we study the relative contribution of bending/axial deformation modes and the cohesion of fibers to the overall mechanical behavior of sparsely cross-linked fiber networks. These are complex multibody systems with highly non-linear mechanics. Their modeling and simulation raises important problems. For example, the fibers bundle and rearrange dynamically even in the unloaded state. Loading changes the degree of bundling and introduces anisotropy. To capture this behavior in models, it is necessary to track the evolution of the bundle sizes and lengths of segments stabilized by cohesion. We develop computational methods able to handle this complexity. The bundling of fibers is simulated in a FEM framework by applying linear kinematic constraints on the fiber network's mesh to make the bundled fibers come together and stick to each other. This involves identification of essential nodes on an initial stress-free fiber network that would be required for applying the kinematic constraints in a consistent manner. These essential nodes are classified or grouped as per their role in the constraining process. Subsequently, adequate linear kinematic constraint for a node is specified based on its classification. Thereafter, additional nodes are generated for mesh refinement, which are not involved in any constraint equations. This talk will address these and related computational issues.

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Title: Anderson-Accelerated Spatial Coupling of Lattice Boltzmann and Navier-Stokes Solvers

Author(s): *Philipp Neumann, *University of Hamburg*; Benjamin Uekermann, *Technical University of Munich*.

Both Lattice Boltzmann (LB) and (incompressible) Navier-Stokes (NS) solvers come with advantages and disadvantages. LB methods provide accurate prediction of fluid flow over a wide range of temporal and spatial scales, including scenarios of fluctuating hydrodynamics and finite Knudsen flow. From the algorithmic perspective, LB is rather simple and very local in its computations. This allows for very efficient and massively parallel simulations on cluster and GPU environments. Incompressible NS solvers typically come with lower memory consumption requirements. They often allow the use of coarser grids and rigorous higher-order discretizations such as discontinuous Galerkin approaches which are rather uncommon in the LB framework. Hence, LB or NS, or a combination of both to exploit their features to highest extent may be favorable for a particular flow problem. In this contribution, I present methods to spatially couple LB and NS solvers for both steady-state [1] and transient [2] simulations. I discuss the mapping of unknowns at the solver interfaces and show validation results from various numerical experiments (channel, Taylor-Green, and Couette flow). I further point out parallelization aspects in the coupled simulation. In particular, I focus on Anderson-accelerated coupling of LB and NS. The Anderson-acceleration technique has gained much interest amongst others in recent partitioned fluid-structure interaction simulations [3] due to the simultaneous execution of the involved solvers. The latter yields additional flexibility of the coupled system with regard to parallelization and respective resource allocation on modern supercomputers. Our coupled LB-NS simulations suggest that the method yields speed ups of up to 40% compared to strictly sequential Schwarz coupling. References: [1] A. Atanasov, B. Uekermann, C.A. Pachajoa Mejía, H.-J. Bungartz, P. Neumann. Steady-State Anderson Accelerated Coupling of Lattice Boltzmann and Navier-Stokes Solvers. Computation 4(4): 1-19, 2016 [2] P. Neumann. On Transient Hybrid Lattice Boltzmann-Navier-Stokes Simulations. Journal of Computational Science 17:482-490, 2016 [3] D. Blom, T. Ertl, O. Fernandes, S. Frey, H. Klimach, V. Krupp, M. Mehl, S. Roller, D.C. Sternel, B. Uekermann, T. Winter, A. van Zuijlen. Partitioned Fluid-Structure-Acoustics Interaction on Distributed Data: Numerical Results and Visualization. In: H.-J. Bungartz, P. Neumann, W.E. Nagel (eds.) Software for Exascale Computing - SPPEXA 2013-2015. Lecture Notes in Computational Science and Engineering 113, 267-291, 2016

14th U.S. National Congress on Computational Mechanics
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Title: Numerical Assessment of Jointed/Faulted Caprock Integrity During CO2 Sequestration

Author(s): *Pania Newell, *The University of Utah*; Mario Martinez, *Sandia National Laboratories*.

Deep geological saline formations have the potential to be considered as permanent/semi-permanent storage units for storing carbon dioxide over long period of 10^3-10^4 years. However, their overall performance depends on the structural trapping mechanism of caprock. This trapping mechanism can be influenced by newly-formed and pre-existing fractures and faults across many scales. The growth and reactivation of these fracture networks are mainly pore pressure driven and are aided by chemical-mechanical interactions. The magnitude of the pressure change not only depends on the hydrological and geomechanical properties of the formations, but also the orientation of the wellbore. In this study, we investigate the impact of formation thickness, wellbore orientation, injection rate and fault(s) on understanding caprock performance during CO2 sequestration. We adopt an equivalent continuum approach to couple geomechanical and reservoir flow response. The results show that higher injection rates independent from wellbore orientation would lead to fracture reactivation within the caprock formation. Additionally, vertical wells lead to higher reservoir pressure changes compared to horizontal injection wells under the same injection rate. We also show that the formation thickness plays an important role in overall performance of the system. For instance, the caprock integrity can be compromised when a thin reservoir overlain by a thin caprock layer compared to a think reservoir overlain by a thick caprock layer subjected to the same injection rate. Impermeable faults can also enhance the activation of the pre-existing fracture leading to higher leakage to the upper surfaces. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
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Title: Isogeometric Analysis for Nonlinear Bending of Microplates

Author(s): *Hoang Nguyen, Thuc Vo, *Northumbria University*.

This study aims to investigate the geometrically nonlinear behaviours of rectangular and circular functionally graded (FG) microplates with size-dependent effects using isogeometric analysis (IGA) approach. While modified couple stress (MCS) theory is introduced to account for small-scale effects, the displacement fields are described based on the four-variable refined plate theory (RPT). The MCS, which has advantages of including asymmetric couple stress tensor and using only one material length scale parameter, would be able to effectively capture the size-dependent effects in nano/micro structures. The RPT, which requires C1 elements, not only is able to improve the accuracy of the analysis but also helps to describe the nonlinear distribution of shear stress through plate thickness without using shear correction factors. The geometrically nonlinear behaviours of rectangular and circular FG microplates based on these two theories are studied in the platform of IGA. This recently developed method utilises the non-uniform rational B-splines (NURBS) functions to establish approximation functions and describe geometry domains simultaneously. In addition, NURBS functions, by its nature, could satisfy high-order continuity which is essentially required in RPT theory without any difficulty. While the governing equations and weak forms are directly derived using Hamilton's principle, the Newton-Raphson iterative algorithm is employed to solve the nonlinear problems. A number of numerical examples conducting for rectangular and circular FG microplates reveal that the consideration of small-scale effects is followed by the increase in plates' stiffness.

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Title: Matching Boundary Conditions for State Based and Bond Based Peridynamics

Author(s): *Clint Nicely, Dong Qian, *University of Texas at Dallas*.

A Matching Boundary Condition (MBC) is presented in this paper for treating the numerical interface in coupling peridynamics (PD) with a continuum simulation based on finite element or meshfree method. The MBC is cast in the form of a parameterized expression that involves the displacements and their higher-order time derivatives of peridynamic (PD) nodes at the numerical interface. The corresponding parameters are solved by enforcing that the dispersion relations obtained from three versions of PD, i.e., bond-based (BBPD), ordinary peridynamics (OPD), and non-ordinary peridynamics (NOPD). Comparisons are made to the MBC implementation in classical Molecular Dynamics (MD). It is found that BBPD is very similar to MD. On the other hand, it is shown that a non-local treatment needs to be introduced for both ordinary and non-ordinary peridynamics for the MBC to be fully effective. Extensive numerical examples in 1D and 2D are presented to validate the robustness of the methods. X. Wang and S. Tang, “Matching boundary conditions for lattice dynamics,” Int. J. Numer. Methods Eng., vol. 93, no. 12, pp. 1255–1285, Mar. 2013. W. Jiang, S. Tang, X. Wang, and D. Qian, "Generalized Matching Boundary Conditions Based on Fourier Transform Technique," Journal of Nanomechanics and Micromechanics, vol. 4, p. A4013011, 2014.

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Title: Adjoint-Based Sensitivity Analysis and Design of Large-Scale Multidisciplinary Aerospace Applications

Author(s): *eric nielsen, *nasa langley research center*.

An overview of current capabilities for adjoint-based sensitivity analysis as applied to multidisciplinary aerospace applications is presented. The general approach for developing the discrete formulation is shown, as well as a verification of the implementation. Challenges related to high-performance computing and other aspects of the simulations will also be shared.

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Title: Kirchhoff-Love Shell Finite Elements Based on Shallow Shell Theory

Author(s): *Antti H. Niemi, *University of Oulu*; Tom Gustafsson, *Aalto University*.

Rotation-free shell finite elements are presented. The formulations are based at the element level on a refined shallow shell model and can be used to model arbitrary doubly-curved shells. The employed shell theory is of Kichhoff-Love type and an assumed strain approach is used to circumvent membrane locking. The relative accuracy and efficiency of the formulations is evaluated in challenging benchmark tests featuring different shell deformation types and compared with analogous Reissner-Mindlin type formulations [1]. [1] Niemi, A. H. Benchmark Computations of Stresses in a Spherical Dome with Shell Finite Elements. SIAM Journal on Scientific Computing 38, B440–B457 (2016).

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Title: A Finite Element Method for the Jones Eigenmodes of an Elastic Scatterer

Author(s): *Nilima Nigam, *Simon Fraser University*.

D.S. Jones, whilst studying the unique solvability of time-harmonic fluid-structure interaction problems for linearly elastic scatterers in fully lubricated contact with their surroundings, observed the possibility of elastic eigenmodes which have zero traction and zero displacement in the normal direction on the boundary of the scatterer. These modes are now termed 'Jones modes'. Not much is known about these modes, or even if they exist for all bounded simply connected scatterers. In this talk, we provide analytical constructions of these eigenmodes in some domains. We also present a novel finite element strategy for these eigenmodes.

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Title: A Fixed Cartesian Mesh Method for Large-Scale Parallel Simulation of Complex Vehicular Structures

Author(s): *Koji Nishiguchi, Rahul Bale, *RIKEN AICS*; Shigenobu Okazawa, *University of Yamanashi*; Makoto Tsubokura, *Kobe University*.

We propose a novel numerical method suitable for large-scale parallel simulations of complex vehicle structure. For the last several decades, a Lagrangian finite element method has been the de facto standard for structure simulations. This method can track the surface of structures with high accuracy and compute constitutive relation of structure with ease, since a geometric domain of the structure is spatially discretized using unstructured mesh which conforms to the deforming structure. However, compared to structured/unstructured Cartesian meshes, the parallel efficiency of the unstructured meshes is limited. With the growing interest in and need of large-scale parallel simulations of vehicle dynamics, there has been a renewed interest in structured/unstructured Cartesian meshes. Furthermore, unstructured mesh generation for complex geometries is a time-consuming process and requires special know-how in general. Considering the above background, we propose a novel simulation technique for vehicle structure dynamics. Our method is based on a hierarchical Cartesian mesh called the building cube method (BCM) [1], which is capable of achieving high parallel efficiency and generating meshes for complex geometry without special know-how. In the BCM, a computational domain is divided into building blocks of cuboids, named Cube, of various sizes to effectively capture complex geometries. In our method, the basic equations of structure are computed in the Eulerian frame [2] because computational mesh is fixed in space. The basic equations are solved using a fractional step method, where the equations are discretized in time using the Adams-Bashforth method and in space using a collocated finite volume method. The VOF method is applied to capture material interfaces and the advection equation of the VOF function is computed with the fifth-order WENO scheme. In my presentation, some simulation examples of vehicular structure will be demonstrated to validate the proposed approach. References: [1] K. Nakahashi, Building-cube method for flow problems with broadband characteristic length, Computational Fluid Dynamics 2002, pp. 77-81, Springer Berlin Heidelberg, 2003. [2] D. J. Benson, Computational methods in Lagrangian and Eulerian hydrocodes, Computer methods in Applied mechanics and Engineering, 99(2-3), 235-394, 1992.

14th U.S. National Congress on Computational Mechanics
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Title: Assessment of Enriched Finite Element Discretizations for Weak Discontinuities

Author(s): *David Noble, *Sandia National Laboratories*; Kurt Maute, *University of Colorado, Boulder*.

Enriched finite element methods are powerful tools for multiphase and multimaterial problems. These methods provide discretizations that dynamically adapt to the moving material and phases to accurately capture the interfacial physics and discontinuities. In order to allow for a discontinuous description across interfaces, these methods introduce some type of enrichment in the elements that are crossed by these interfaces. Additional unknowns are assigned to one or more of the mesh entities (elements, nodes, sides, or edges) that are associated with these interfacial elements, and additional equations are formulated for these unknowns. The Conformal Decomposition Finite Element Method (CDFEM) is an enriched finite element method that can be used to describe arbitrarily discontinuous physics across dynamic interfaces. Level sets are used to describe the location of the moving interfaces. Nodes are added at the intersection of the level set surfaces with the edges of the input mesh, and a conforming mesh is generated automatically. Standard unstructured mesh data structures are generated for the resulting conformal mesh in terms of element blocks and side sets. This general framework allows the physics code to describe either weak or strong discontinuities across the interfaces using standard finite element methods. Criticism of CDFEM has focused on two issues. First, the resulting conformal mesh may have arbitrarily poor quality. Second, the system of equations produced by such a discretization may have an unbounded condition number. Work in the past has shown that, despite these criticisms, the method produces optimal orders of convergence in both the L2 norm and H1-seminorm. It has also been observed that it is possible to recover a Heaviside enriched discretization from a CDFEM discretization by constraining the degrees of freedom at the added nodes to the Heaviside enriched space of functions. In this way CDFEM can be viewed as a preprocessing step. The mesh is decomposed into elements that conform to the implicit, level set interface. The system of equations on this conformal mesh are assembled. Constraints are formed where the added nodal degrees of freedom are specified in terms of Heaviside enriched degrees of freedom. The solution of this constrained system is identical to that obtained by directly assembling the Heaviside enriched system of equations. In this talk, the accuracy and solvability of multiple enriched discretizations is assessed. A simple scalar diffusion problem with an embedded weak discontinuity is used as a testbed. Three discretizations are assessed: CDFEM, a Heaviside enriched discretization with Nitche-type compatibility conditions, and a simple, piecewise linear enriched discretization with weak discontinuity support. The accuracy of the solutions is quantified. Also, the condition number of the resulting system of equations is quantified. This assessment shows the relative strengths and weaknesses of each method. *Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Curved-Plate Structures with Placement Bounds

Author(s): Shanglong Zhang, *Julian Norato, *University of Connecticut*.

Single curvature plates are commonly encountered in mechanical and civil structures, particularly those fabricated by joining of bent plates. In this presentation, we introduce a topology optimization method for the stiffness-based design of structures made of curved plates with fixed thickness. The geometry of each curved plate is analytically and explicitly represented by its location, orientation, dimension and curvature radius. These variables constitute the design parameters for the optimization, and therefore the method renders designs that are distinctly made of curved plates that can be manufactured by joining bent stock plates. To perform the primal and sensitivity analyses, we employ the geometry projection method, which smoothly maps the analytical geometry of the curved plates onto a continuous density field defined over a fixed uniform finite element grid. In addition to the aforementioned geometric variables, a size variable is ascribed to each curved plate and penalized in the spirit of solid isotropic material with penalization (SIMP) so that the optimizer can entirely remove a curved plate from the design when its size variable attains a near-zero value. The main advantage of our method is to produce designs that are solely made of curved plates. However, our method retains two significant advantages that existing free-form topology optimization techniques exhibit: 1) we circumvent re-meshing upon design changes by projecting the geometries of the curved plates onto a fixed finite element grid and using an ersatz material model for the analysis; and 2) the differentiability of the projection and the chain rule allow the utilization of efficient gradient-based optimization methods. In addition to these benefits, the explicit representation of the curved plates provides a direct translation of the optimum design into a computer-aided design model. In this work, we also make an additional consideration with regards to manufacturability: we impose placement bounds on the curved plates to ensure the entire plate remains inside of the design envelope. By doing this, we avoid optimal designs that would have cuts that are nearly parallel to the main plane of the plate (i.e. the plane perpendicular to the plate thickness), which are very difficult to manufacture. Our method also naturally accommodates designs for plates with given multiple thicknesses. We present numerical examples to demonstrate the applicability of the proposed method.

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Title: An Adaptive Residual Based Approach for Solving the Penalized Navier-Stokes Equations in Fluid Structure Interaction

Author(s): *Léo Nouveau, *INRIA Bordeaux/Duke University*; Héloïse Beaugendre, Cécile Dobrzynski, *INRIA Bordeaux Sud-Ouest, Bordeaux INP, IMB*; Mario Ricchiuto, *NRIA Bordeaux Sud-Ouest*.

In the context of Fluid Structure Interaction involving rigid bodies, this work proposes to combine an Immersed Boundary (IB) method known as Penalization (introduced by Brinkmann [1]) and the simplicity provided by unstructured grids to perform adaptation. An r-adaptation strategy combined to the use of Arbitrary Lagrangian Eulerian (ALE) framework is employed, avoiding remeshing and interpolation steps. The adaptation is performed defining a monitor function that equidistributes the nodes [2]. We define here the monitor function to allow an adaptation to the solid boundary to accurately impose the Boundary Condition (BC), and to a chosen physical variable to improve the solution accuracy. A second-order Residual Distribution scheme [3] is proposed to solve the ALE equations: an SUPG spatial discretization along with a Crank–Nicolson time discretization. Validations are proposed, with computational time comparisons to prove the efficiency of the proposed approach. Acknowledgments The research leading to these results has received funding from the European Union Seventh Framework Programme FP7/2007-2013 under grant agreement n 605180. References: [1] Brinkman, H.C. A calculation of the viscous force exerted by a flowing fluid on a dense swarm of particles. Appl Sci Res, Vol. 1(1), (1949). [2] Tang, H. and Tang, T. Adaptive Mesh Methods for One- and Two-Dimensional Hyperbolic Conservation Laws. SIAM J Numer Anal, Vol. 41, (2003). [3] Ricchiuto, M. Contributions to the development of residual discretizations for hyperbolic conservation laws with application to shallow water flows. HDR Thesis, (2011).

14th U.S. National Congress on Computational Mechanics
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Title: Progress Towards the Development of a 2D Immersed Boundary Solver for the Simulation of Particles at Fluid-Fluid Interfaces

Author(s): *Adam O'Brien, Markus Bussmann, *University of Toronto*.

Interactions between particles and fluid-fluid interfaces are important in many fundamental studies of industrial processes of interest at the milli- to micro scale. In this work, progress towards the development of an extensible numerical framework for simulating particles at fluid-fluid interfaces is presented. The Immersed Boundary (IB) method is used for the inclusion of particles, with a new model for varying the wettability of the surface. The proposed method of modelling contact lines along an IB surface follows from the CELESTE method of evaluating interface forces (Denner and van Wachem 2014). The method is coupled to a moving sharp-interface IB implementation, allowing for a high resolution representation of the geometry and good mass conservation properties. The flexible use of a least squares method allows for the contact line model to be used with any of the sharp interface IB methods, including ghost-cell methods, cut-cell methods and hybrid schemes, while maintaining a consistent approach to curvature evaluation with respect to the rest of the fluid domain.

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Title: Applications of a Multi-Scale Generalized Finite Element Method to Three-Dimensional Anisotropic Heterogeneous Materials

Author(s): *Patrick O'Hara, *UTC/AFRL*; Piyush Gupta, Haoyang Li, *University of Illinois*; Deniz Ozturk, *Johns Hopkins University*.

P. O'Hara1 , P. Gupta2 , D. Ozturk3 and H. Li2 1 Universal Technology Corporation/AFRL, of Illinois, 3 Johns Hopkins University, 2 University Abstract The ability to accurately and efficiently predict stable crack growth in a structure is currently an active area of research in the civil, mechanical and aerospace communities, and has been for decades. There are many numerical techniques which are available for this class of structural analysis. The methodology investigated in this work is the generalized finite element method (GFEM) [2], which has the primary benefit over stan- dard FE approaches of representing a crack surface independent of the FE mesh itself. The GFEM, and other similar enriched FE approaches have been successfully applied to fracture simulations primarily in the context of isotropic, homogeneous materials. While these material level assumptions hold for a broad range of structural materials, there are certain classes of materials in use which require a more detailed representa- tion of the material itself, particularly grain-driven anisotropy, in order to obtain accurate macro-scale crack growth predictions. It may be noted that the enriched FE approaches which work well for the isotropic case require significant, non-trivial, modification to be made appropriate for anisotropic or heterogeneous mate- rial systems. The essential issue is the lack of availability of an accurate a priori enrichment basis which can be used for this class of problems. The application considered in this work does not lend itself to the practical derivation of a priori enrichment bases. A more general form of the GFEM, known as the GFEM with global-local enrichment functions (GFEM gl) [1] has been developed to alleviate this potential limitation. The GFEM gl uses a small-scale boundary value problem (BVP) in a particular region of localized interest to numerically compute a special- ized enrichment basis corresponding to the localized physics of interest. In the current work, the small-scale BVP consists of a highly-adapted localized region of anisotropic elastic grains containing mechanically- short cracks with the goal of investigating how the local material heterogeneity influences the near-tip stress fields in the body. While the ultimate goal is to predict crack propagation trajectories in heterogeneous ma- terials, the current work is restricted to static fracture scenarios, and accuracy of the approach is assessed via comparison with solutions generated on overkill meshes utilizing the standard hp-GFEM. References [1] C.A. Duarte and D.-J. Kim. Analysis and applications of a generalized finite element method with global-local enrichment functions. Computer Methods in Applied Mechanics and Engineering, 197 (6-8):487–504, 2008. doi: 10.1016/j.cma.2007.08.017. [2] C.A. Duarte, I. Babuška, and J.T. Oden. Generalized finite element methods for three dimensional structural mechanics problems. Computers and Structures, 77:215–232, 2000. doi: 10.1016/S0045- 7949(99)00211-4.

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Title: Goal-Oriented Mesh Adaptation Enabled by the Variational Multiscale Method

Author(s): Brian Granzow, *Assad Oberai, *RPI*.

In the variational multiscale (VMS) method, the solution to a given problem is split into coarse and fine scale components. Thereafter, a simplified representation for the fine scales, driven by the residual of the coarse scales is derived, and used in the equation for the coarse scales. This yields an improved formulation for the coarse-scale solution. When estimating the error in a quantity of interest (QoI) that depends on this solution, it is natural to consider this fine scale component as the error in the solution, and use it to directly estimate the error in the QoI. We refer to this estimate of the error in the QoI as the “direct” estimate. In contrast to this, the standard approach to estimating the error in a QoI, which applies to any numerical method, involves formulating and solving an auxiliary dual problem, and weighting the residual of the original primal problem by the dual solution, in order to estimate the error. For this approach to yield useful results, the dual problem must be solved using an enriched basis. An alternative, which is considered here, is to apply the VMS method to the dual problem and use the fine-scale component of the dual as the enrichment. This leads to an “indirect” application of the VMS method to estimating error in the QoI. In this talk we prove that (remarkably) both the direct and indirect approaches to error estimation lead to the same global error estimate for the QoI. However, the indirect approach leads to a much more useful local estimate of the error, which is necessary to drive mesh adaptation. We demonstrate this through some interesting numerical examples. This talk is based on joint work with Mark Shephard. Thank you Mark for your inclusiveness and your insights. Best wishes on your birthday!

14th U.S. National Congress on Computational Mechanics
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Title: Selection, Calibration, and Validation of Predictive Multiscale Models of Tumor Growth

Author(s): *J. Tinsley Oden, Ernesto Lima, *The University of Texas at Austin*; Thomas Horger, Barbara Wohlmuth, *Technical University of Munich*; Amir Shahmoradi, David Hormuth, Thomas Yankeelov, *University of Texas at Austin*.

The concept of predictive computational medicine has gradually emerged in recent years as a new paradigm of medical science in which patient-specific predictions and diagnoses are made use high-fidelity computational models of the behavior of living organisms (see, e.g. [1,2,3]). Such approaches are in stark contrast to traditional medicine, which relies on statistical trends based on data taken from large populations of patients, and in vitro laboratory tests. But, the success of predictive computational methods requires that uncertainties in observational data, model selection, model parameters, and predictions of therapeutic outcomes be carefully assessed and quantified. It is, in some respects, data driven, as relevant observational data is necessary to calibrate, select, and, ultimately, validate models in the presence of often confounding uncertainties, but the selection and validation of predictive computational models is an issue of overriding importance. This presentation covers the development of predictive multiscale computational models of tumor growth in living organisms at the tissue, cellular, and sub-cellular (protein signaling) scale set in a general Bayesian framework, with also an appeal to information theory and entropy methods. A large family of parametric model classes is developed based on a combination of continuum mixture theory and well-established principles of cancer biology. MRI data on glioma in laboratory animals is accessed to guide Bayesian methods for model calibration, selection and validation using a version of the OPAL algorithm [4]. Results on three-scale interactions of stochastic models of cell proliferation and signaling pathways are presented. Encouraging predictions of tumor mass evolving in laboratory animals and of the effects of radiation therapy are discussed. References: 1. Oden, J.T.; Lima, E.A.B.F.; Almeida, R.C.; Feng, Y.S.; Rylander, M.N., Fuentes, D.; Faghihi, D.; Rahman, M.M.; DeWitt, M.; Gadde, M.; and Zhou, J.C. “Toward predictive multiscale modeling of vascular tumor growth,” Archives of Computational Methods in Engineering, DOI10.1007/s 11831-015-9156-x, 2015. 2. Oden, J.T. “Foundations of Predictive Computational Science”, ICES-17- January 5, 2017 3. Lima, E.A.B.F.; Oden, J.T.; Hormuth, D.A.; Yankeelov, T.E.; and Almeida, R.C. “Selection, calibration, and validation of models of tumor growth”, Math. Models Methods Appl. Sci. 26, 2341, 2016. 4. Farrell, K.; Oden, J.T.; and Faghihi, D. “A Bayesian framework for adaptive selection, calibration, and validation of coarse-grained models of atomic systems,” Journal of Computational Physics, v. 295, pp. 181-208, 2015.

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14th U.S. National Congress on Computational Mechanics
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Title: OPAL: Bayesian Framework for Model Selection and Quantifying Model Inadequacy

Author(s): *J. Tinsley Oden, Ernesto Lima, Amir Shahmoradi, David Hormuth, Thomas Yankeelov, *University of Texas at Austin*; Barbara Wohlmuth, Thomas Horger, *Technical University of Munich*.

Every step in the process of developing computer predictions of natural events inevitably encounters uncertainties: uncertainties in the observational data, in model selection, in model parameters, and in the quantification of the target quantities of interest. An issue of special concern is the validity of models used in the prediction and the quantification of inevitable model inadequacy. In this presentation, we discuss OPAL: The Occam Plausibility Algorithm, as a systematic approach to model selection and validation in the presence of uncertainties. Applications are given for multiscale models of tumor growth in laboratory animals. The notions of Bayesian posterior model plausibilities, maximum entropy priors, model inadequacy and validation, and solutions of systems of stochastic pde's are discussed, and specific applications are described.

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14th U.S. National Congress on Computational Mechanics
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Title: A Variational Method to Avoid Locking – Independent of the Discretization

Author(s): *Bastian Oesterle, *Inst. for Str. Mech., UofSt*; Simon Bieber, Ekkehard Ramm, Manfred Bischoff, *Institute for Structural Mechanics, University of Stuttgart*.

Since the pioneering contribution by Hughes and co-workers in 2005 [1], isogeometric methods received a great deal of attention in academia and industry. Besides promising results in a wide range of problems, standard isogeometric finite elements still suffer from the same locking effects as classical finite elements. Hierarchic formulations, as presented in [2], lead to purely primal plate and shell formulations, intrinsically free from transverse shear locking, independent of the discretization. A corresponding primal formulation to avoid membrane locking has not yet been found. Element formulations based on mixed methods also present very promising candidates to avoid the various locking phenomena present in (isogeometric) finite elements ([2], [3]). The major task in their development is the thorough choice of the corresponding stress or strain spaces. Too rich spaces do not fully remove locking, too poor spaces may introduce spurious modes. Furthermore, the choice of balanced stress/strain spaces usually requires several different (lower) spaces for their discretization. However, different spaces are neither efficient, nor “isogeometric”. In addition, they are restricted to only one discretization, and the extension to advanced smooth discretization schemes like T-Splines, subdivision surfaces or meshless methods are either very complicated or hardly possible. In this contribution, we present a new, unified concept to develop mixed finite elements, independent of the underlying discretization scheme. In particular, we present locking-free finite element formulations for continua, plates and shells, discretized by several different schemes like standard finite elements, isogeometric finite elements based on NURBS and meshless methods based on maximum-entropy approximants. References [1] T. J. R. Hughes, J. A. Cottrell, Y. Bazilevs, Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement, Computer Methods in Applied Mechanics and Engineering 194: 4135–4195, 2005. [2] R. Echter, B. Oesterle, M. Bischoff. A hierarchic family of isogeometric shell finite elements. Computer Methods in Applied Mechanics and Engineering, 254: 170–180, 2013. [3] T. Elguedj, Y. Bazilevs, V. M. Calo, T. J. R. Hughes, Bbar- and Fbar- projection methods for nearly incompressible linear and non-linear elasticity and plasticity using higher-order nurbs elements, Computer Methods in Applied Mechanics and Engineering 197: 2732–2762, 2008.

14th U.S. National Congress on Computational Mechanics
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Title: Maximization of Energy Absorption Capacity Applying Elastoplastic Multi-Scale Topology Optimization

Author(s): *Shun Ogawa, Hiroya Hoshiba, Junji Kato, Takashi Kyoya, *Tohoku University*.

The present study proposes topology optimization of microstructure considering nonlinear structural responses at micro and macro levels. It is assumed that the microstructure consists of a two-phase material based on elastoplastic von Mises model. Only one microstructure is allowed over the entire region of the macrostructure, namely uniformly-structural material. The energy absorption capacity of the macrostructure is chosen as the objective function, and its performance is maximized under a prescribed material volume of constituents. The design variable is defined as the volume fraction of each finite element in a unit cell. A decoupling multi-scale analysis based on homogenization is used to solve the two-scale BVP. The decoupling multi-scale analysis is known as a method to reduce computational costs by dividing the original BVP into two separate BVPs. For a gradient-based topology optimization, accurate sensitivity analysis is necessary to obtain a reliable optimization result. In this context, the present study proposes sensitivity analysis based on numerical material tests. With this approach, highly accurate sensitivity can be obtained without calculating the implicit sensitivities; this allows a dramatic reduction in the computational efforts. It is verified by a series of numerical examples that the proposed method provides reliable optimization results with moderate computation and has a great potential for advanced material design.

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Title: Efficient Solution of Eigenvalue Problems Related to Coupled Acoustical Systems

Author(s): *Antti Ojalammi, Antti Hannukainen, *Aalto Univesity School of Science, Department of Mathematics and Systems Analysis*.

The motivation for this talk arises from the computation of resonant frequencies in the human vocal tract, which is a central problem in modeling of speech production [1]. Such resonance computations are performed on several vocal tract geometries corresponding to different vowels. A common practice is to assume that the exterior space does not affect the resonances, and to limit the computational domain only to the vocal tract. However, recently performed simultaneous MRI measurements and voice recordings indicate that the exterior space may affect the resonances. Including a realistic exterior space model into the resonance computation greatly increases the size of the resulting system and the required computational time [2]. In this talk, we present a method for reducing the dimension of the finite element matrices related to the exterior space, leading to a considerable speed up in the resonance computations. Mathematically, we are interested in computing the eigenvalues of the Laplace operator on a pre-specified interval. When the exterior space is included into the finite element simulation, the computational domain consists of two parts: the vocal tract and the exterior space. The interface between these two subdomains is located at the mouth. We assume that the exterior space does not change between different geometries and simulations. The eigenvalue problem is discretized using a finite element method. To avoid technical difficulties in mesh generation, Nitsche's method is used on the interface to connect the possibly non-matching vocal tract and exterior meshes. Achieving sufficient accuracy requires considerably more degrees of freedom in the exterior space in comparison to the vocal tract. The proposed method greatly reduces the computational cost of solving eigenvalues that lie on the specified interval. The reduction is based on constructing a special basis for the exterior domain. The basis is constructed by solving a set of auxiliary problems related to the exterior space and compressing the resulting solution set using SVD. The efficiency of the presented method is demonstrated on numerical examples. In addi- tion, we give an outline of the error analysis, which can be done in the subspace projection method framework. References: [1] Hannukainen, A., Lukkari, T., Malinen, J. & Palo, P. Vowel formants from the wave equation. J. Acoust. Soc. Am. 122, EL1–EL7 (2007). [2] Hannukainen, A., Ojalammi, A. & Malinen, J. Exterior space model for an Acoustic Eigenvalue Problem. In Proceedings of 27th Nordic Seminar on Computational Mechanics, 85–88 (2014).

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Title: Evaluation of J- and Interaction Integrals for Fracture Problems of Welded Joints

Author(s): *Hiroshi Okada, Masahiro Ono, Koichiro Arai, Yasunori Yusa, *Tokyo University of Science*.

In this presentation, we discuss about methodologies to perform fracture mechanics analysis on welded joints. Welding involves many thermal/mechanical/physical phenomena. The fracture problems of welded joints are associated with complex residual stress distribution, with spatial change of mechanical properties of material and with dissimilar material interfaces. Furthermore, a welded joint may experience large deformations before its fracture. Fracture mechanics analysis on welded joints involves many challenges in terms of computational fracture mechanics, namely, (1) Finite element model generation: In present investigation, automatic mesh generation scheme with tetrahedral finite element is adopted to overcome this problem; (2) Residual stress/spatial variations in material properties: The residual stresses and spatial variations in material properties need to be taken into consideration in the computations of the J-integral and the stress intensity factors; (3) The effects of large deformation need to appropriately be considered in the evaluation of the J-integral. To overcome the difficulties that are involved in items (2) and (3), additional terms are added to the formulations of the domain integral method. The additional terms involve the spatial derivatives of the strain energy density and the displacement gradients that are evaluated at the integration points of the finite elements. In our presentation at USNCCM14, we will address the formulae of the J-integral and the interaction integral, how we can compute them numerically and some remaining problems. Acknowledgement: Research performed by H.O. has been supported by JSPS (Japan Society for the Promotion of Science) Grant-in-Aid for Scientific Research (C) No.16K05988. The support is gratefully acknowledged.

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Title: Adaptive Isogeometric Analysis of Thin Plate Problems using Recovery-Based Error Estimation

Author(s): *Knut Morten Okstad, Trond Kvamsdal, *SINTEF Digital*; Mukesh Kumar, *College of Charleston*; Kjell Magne Mathisen, *Norwegian University of Science and Technology*; Terje Haukaas, *University of British Columbia*.

The use of patch recovery techniques in adaptive finite element analysis of linear elasticity and plate problems was demonstrated by the authors in [1] and [2], where the concept of using a special basis for the recovered field that satisfied the balance equation a priori was introduced. Recently, this method was revisited and used in the context of isogeometric analysis. In the current work, we employ this method in isogeometric analysis of structural plate problems and demonstrate its capability on some civil engineering applications. In these applications, one often encounter stress concentrations due to, e.g., the mating of columns and plates, that will require tailoring of the computational mesh to obtain an optimal model. Using adaptive analysis is a way of automating this process. References [1] Kvamsdal, T. and Okstad, K. M. Error estimation based on superconvergent patch recovery using statically admissible stress fields. International Journal for Numerical Methods in Engineering, 42(3), pp. 443-472, 1998. [2] Okstad, K. M., Kvamsdal, T. and Mathisen, K. M. Superconvergent patch recovery for plate problems using statically admissible stress resultant fields. International Journal for Numerical Methods in Engineering, 44(5), pp. 697-727, 1999. [3] Kumar, M., Kvamsdal, T. and Johannessen, K. A. Superconvergent patch recovery and a posteriori error estimation technique in adaptive isogeometric analysis. Computer Methods in Applied Mechanics and Engineering, 316, pp. 1086-1156, 2017.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Tensor-Based Metamodels for the Calibration of Constitutive Laws in Material Science

Author(s): *Clement Olivier, *Safran / Mines ParisTech*; David Ryckelynck, *Mines ParisTech*; Julien Cortial, *Safran*.

Predictive numerical models in material science typically involve highly nonlinear coupled differential algebraic equations and feature up to 20 or more parameters that must be appropriately calibrated to mimic the actual physical behavior. However, defining unambiguous criteria measuring the fidelity of the model to experimental data is a challenging task. First, the model may be imperfect and unable to reproduce some observed physical behaviors. Second, experimental data is marred by uncertainties such that the calibration of the model amounts to find a range of admissible parameter values for which the corresponding numerical results are comprised in an experimental confidence interval. As a result, the closely related processes of identification and validation require a strong human expertise whose scarcity is incompatible with the long response times of sophisticated but computationally expensive numerical models. A common technique is to rely on a surrogate model that maps the input parameters to the outputs of interest and is extremely cheap to evaluate compared to the original model. A two-phase strategy is adopted: The training phase is dedicated to the assimilation of empirical data obtained by exercising the reference model, while the exploitation phase consists in calling the resulting approximate model in a way that would be unaffordable otherwise. This approach is applicable to many types of analyses such as model calibration as stated above, but also parametric sensibility estimation or uncertainty quantification. The method developed in the present work relies on a key insight underlying the Proper Generalized Decomposition (PGD) to construct surrogate models, namely the interpretation of the set of all possible parameter dependent solutions as a multidimensional tensor. Unlike the PGD that uses the well-known canonical decomposition, the recently introduced tensor train decomposition (TT) is at the heart of the proposed metamodel. The training phase, based on a variant of the TT-cross algorithm, consists in building simultaneously, for a given level of accuracy, approximations for all heterogeneous quantities of interest that are valid over a large parameter domain. A parsimonious exploration of the parameter space enables to keep the computational effort reasonable. The application to nonlinear constitutive laws shows that the error level between the surrogate and physical model is sufficiently low to perform parametric studies such as identification. The potential of the methodology is also illustrated by an interactive visualization tool enabling the real-time exploration of the model over the parameter space.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Blended Force-Based Quasicontinuum Method for Multilattice Materials

Author(s): *Derek Olson, *RPI*; Xingjie Li, *UNC-Charlotte*.

Blended atomistic-to-continuum methods operate by smoothly blending atomistic and continuum forces (or energies) over a blending, or transition region. In this talk, we present the blended force-based quasicontinuum (BQCF) method for defects in multilattices and state rigorous error estimates for the method in terms of computational complexity. We verify these estimates by applying the method to a Stone-Wales defect in a single layer of graphene, and then we describe how certain bilayer materials can be modeled within the existing framework of the multilattice BQCF method. We discuss the limitations in doing so and some of the challenges involved.

14th U.S. National Congress on Computational Mechanics
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Title: Early Detection of Breast Cancer through an Inverse Problem Approach to Stiffness Mapping: Preliminary Results from Tissue Phantom Experiments

Author(s): *Lorraine Olson, Robert Throne, Adam Nolte, Kaelyn Griffin, Nicolae Iovanac, Xiaoyin Ling, Tressa Lauer, Michael Samp, Brendan Smyth, Jiaojiao Wang, *Rose-Hulman Inst of Tech*.

Early detection of breast cancer will continue to be crucial in improving patient survival rates. Manual breast exams and mammograms are the most widely used early detection techniques. Unfortunately, manual breast exams are limited in their ability to detect tumors since they only produce qualitative information about the site where the force is applied. Mammograms, while effective, expose the patient to radiation and hence routine mammograms are limited to specific risk groups. In addition, mammograms do not quantify tissue stiffness, an identifying characteristic of breast tumors. Our ultimate goal is to develop a system that exploits this stiffness difference to automate, quantify, and enhance the resolution of the manual breast exam. An electro-mechanical device will gently indent the tissue surface in various locations, recording tissue surface deflections on the remainder of the surface. This deflection data will be used with inverse techniques involving finite element methods (FEM) and genetic algorithms (GA) to provide 3D maps of the elastic modulus of the interior of the breast tissue to identify suspicious sites. These maps could also provide quantitative values for comparing baseline data with data taken on subsequent visits, providing yet another mechanism for early identification of cancerous sites. We have developed appropriate computational algorithms and examined their performance extensively on two- and three-dimensional model problems. A variety of tumor locations were assumed, and numerical "measured results" were created with noise added to simulate measurement errors. We found that tumors as small as 1 cm could be detected reliably for these simplified test cases. Much of our recent work focuses on experimental validation. The experiment consists of three stages: 1) Phantom creation and characterization - create gelatin tissue phantoms with and without tumors 2) Indentation experiments - measure surface displacements on tissue phantoms undergoing indentation 3) Data postprocessing - use the GA/FEM to identify tumor locations Preliminary results are quite promising. To date, we have tested five tumor-free phantoms and three phantoms with 2g tumors. In all cases the algorithm was able to identify the presence or absence of a tumor. In addition, the identified tumor locations were appropriate. Acknowledgements: We wish to thank Michael Insana (University of Illinois) for his advice and support. This work is based upon work supported by NSF grant ECCS-1306808, and used the Extreme Science and Engineering Discovery Environment (XSEDE) which is supported by NSF grant OCI-1053575.

14th U.S. National Congress on Computational Mechanics
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Title: Computational, Three-Dimensional Investigation of Endocytosis

Author(s): *Yannick A. D. Omar, Roger A. Sauer, *RWTH Aachen University*; Kranthi K. Mandadapu, *University of California Berkeley*.

Endocytosis is a process in which cells form invaginations by internalizing parts of the plasma membrane for the purpose of bringing cargo into the cell. It is an important means to transport material into cells. In particular, the cargo can be various proteins but also pathogens. Endocytic events can be mediated through a clathrin coat attaching to the lipid bilayer of the cell. The protein's structure induces curvature into the lipid bilayer, thus forming an invagination and subsequently a bud that carries the material to be transported into the cell. When the bud is sufficiently constricted, scission occurs at the bud's neck and a clathrin-coated vesicle is formed. In vivo, the process includes a manifold of factors that may influence the outcome, e.g. actin-induced forces, BAR-proteins and turgor pressure. Despite the fact that clathrin-mediated endocytosis has been studied extensively, its mechanics are not yet fully understood. Lipid Bilayers are part of the outer boundary of cells. Lipid Bilayers are usually modeled as liquid shells based on the Helfrich Hamiltonian. A liquid shell does not have any shear resistance in its in-plane direction. There are few non-axisymmetric, continuum simulation studies on lipid bilayers available. Recent findings for lipid bilayers based on a three-dimensional, C1-continuous Finite Element formulation suggest that non-axisymmetric solutions may be energetically preferable (Sauer et al., 2017). However, to the best of the authors' knowledge, there does not exist a systematic investigation of the effect of the various material and load parameters affecting endocytosis in a general, three-dimensional set-up. Therefore, results comparing axisymmetric and non-axisymmetric solutions on different geometries will be presented to indicate the effect of various factors such as the bending modulus, surrounding surface tension and viscosity. Further, some model limitations and modeling aspects such as area compressibility and shear stabilization will be discussed. Sauer, R. A., Duong, T. X., Mandadapu, K. K., and Steigmann, D. J. (2017). A stabilized finite element formulation for liquid shells and its application to lipid bilayers. J. Comput. Phys., 330:436-466

14th U.S. National Congress on Computational Mechanics
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Title: F-bar Aided Edge-Based Smoothed Finite Element Method with 4-Node Tetrahedral Elements for Viscoelastic Large Deformation Problems

Author(s): *Yuki Onishi, *Tokyo Institute of Technology*.

Accuracy of the recent advanced smoothed finite element formulation for 4-node tetrahedral (T4) elements, F-barES-FEM-T4 [1], in large deformation problems of viscoelastic materials are demonstrated. There are a lot of advantages in F-barES-FEM-T4: shear/volumetric locking free, less corner locking, no increase in DOF, extensibility to dynamic explicit scheme and so on. Among them, the biggest advantage of F-barES-FEM-T4 is the suppression of pressure checkerboarding in nearly incompressible materials even with the use of T4 elements. Nearly incompressibility appears not only in hyperelastic cases but also in elastoplastic or viscoelastic cases. Our group recently confirmed that F-barES-FEM-T4 had very low pressure checkerboarding in hyperelastic and elastoplastic large deformation problems, but did not in viscoelastic problems yet. This study introduces the viscoelastic material based on the generalized Maxwell model to the time-dependent quasi-static formulation of F-barES-FEM-T4. Some examples of viscous analysis reveal that F-barES-FEM-T4 inherits all the advantages including the suppression of pressure checkerboarding even when the long-term Poisson's ratio exceeds 0.49. References: [1] Y. Onishi et al., "F-bar aided edge-based smoothed finite element method using tetrahedral elements for finite deformation analysis of nearly incompressible solids", Int. J. Numer. Meth. Engng, 2017; 109 (11): 1582-1606.

14th U.S. National Congress on Computational Mechanics
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Title: Recent Advances in Numerical Integration in Meshfree Galerkin Methods

Author(s): *Alejandro Ortiz-Bernardin, *Universidad de Chile*.

Over the past two decades, meshfree methods have undergone significant development as a numerical tool to solve partial differential equations (PDEs). In contrast to finite elements, the basis functions in meshfree methods are smooth (nonpolynomial functions), and they do not rely on an underlying mesh structure for their construction. These features render meshfree methods to be particularly appealing for higher-order PDEs and for large deformation simulations of solid continua. However, a deficiency that still persists in meshfree Galerkin methods is the inaccuracies in numerical integration, which affects the consistency and stability of the method. Existing integration schemes for meshfree Galerkin methods tackle the issue of integration errors with an eye on consistency, but without explicitly ensuring stability. In this talk, the combination of meshfree methods and the virtual element method will be presented as a new numerical integration scheme that guarantees both the consistency and stability of the approximate bilinear form in meshfree Galerkin methods.

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Title: Reduced Order Variational Multiscale Enrichment Method (ROVME) for Coupled Thermo-Mechanical Problems

Author(s): Shuhai Zhang, *Vanderbilt University*; *Caglar Oskay, *Vanderbilt University, Nashville, TN, USA*.

We present the formulation and implementation of the reduced order variational multiscale enrichment (ROVME) method for the analysis of inelastic mechanical and coupled thermo-mechanical problems. Based on the variational multiscale enrichment (VME) method, which is a scale-inseparable global-local approach, ROVME method provides an eigenstrain-based model order reduction technique to improve the computational efficiency while maintaining the computational accuracy. It eliminates the requirement of fine scale discretization at subdomains of interest, and upscales the fine scale response to form a single coarse scale (i.e., homogenized) system. The inelastic material behavior is modeled using Perzyna type viscoplasticity and the flow stress evolution is idealized by the Johnson-Cook model. This nonlinear ROVME system is linearized and evaluated using an iterative computational scheme. The ROVME method is extended for coupled thermo-mechanical problems by considering the thermal deformation and temperature dependent material properties. To avoid the repetitive re-evaluation of the temperature sensitive coefficient tensors of the ROVME method, a numerical approach is developed to accurately approximate the coefficient tensors. The key contributions of the presentation are: (1) extending the Eigen-deformation based reduced order modeling method to scale-inseparable problems; (2) improving the convergence rate of the VME method by satisfying the microscale equilibrium automatically; and (3) improving the model order reduction technique to address strongly coupled thermo-mechanical problems. Numerical verifications are performed to assess the accuracy and computational efficiency of the ROVME computational framework, against the fully discretized finite element method and direct VME approach. The performance of ROVME method for coupled thermo-mechanical problems is also tested from different perspectives, such as structures with uniform temperature field, structures with temperature gradient and mechanical loads. The results of the numerical verifications reveal high accuracy and computational efficiency of the ROVME computational methodology.

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Title: Recent Developments and Usage of the Composite Tetrahedral Element in Solid Mechanics Applications

Author(s): *Jakob Ostien, James Foulk III, Alejandro Mota, Michael Veilleux, Nathan Crane, *Sandia National Laboratories*.

Motivated by solving large deformation mechanics problems on non-trivial geometries, including inelastic deformation leading to material failure, extensions to the 10-node tetrahedral element formulation from [1] are presented and discussed. The work showcases a more accurate methodology for capturing the correct volume and assumed linear basis when the mid-edge nodes are not collinear with the major vertex nodes, as when greater geometric fidelity is required. Additionally, in the context of explicit time integration a critical time step estimate is developed and evaluated, mindful of computational efficiency. Emphasis is placed in the evaluation of the element formulation for explicit time integration, in the presence of contact, and in the context of large inelastic deformation. Several application examples will be discussed, demonstrating the accuracy and robustness of the formulation and implementation in a production engineering analysis finite element code. [1] Ostien, J. T., J. W. Foulk, A. Mota, and M. G. Veilleux. "A 10■Node Composite Tetrahedral Finite Element for Solid Mechanics." International Journal for Numerical Methods in Engineering (2016). Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
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Title: Peridynamic Modelling of Pit-To-Crack Transition

Author(s): Dennj De Meo, Luigi Russo, *Erkan Oterkus, *University of Strathclyde*.

Even though the incidence of fatigue loading mainly governs the failure mechanisms in aerospace structures, pit-to-crack transition can still occur in many aluminum alloys, stainless steels and high strength low alloy steels. Despite of the relative rarity of this phenomenon, the consequent failures can be extremely destructive and lead to the loss of an aircraft. In February 1992, a military jet crashed because of a localized corrosion and subsequent stress corrosion cracking (SCC) fracture of the lever-arm-pin in the jet engine made of austenitic stainless steel [1]. Qualitative and quantitative prediction of damage evolution due to corrosion pits acting as precursor to cracking has been hampered by lack of insight into the process, and limitations in visualization and measurement techniques. For long cracks, standards for quantifying environment-assisted crack growth rates can be found. However, in relation to the growth rate of small cracks emerging from corrosion pits, there are no standards available to guide the measurement process. In this regard, numerical modeling can be beneficial. However, the popular assumption that the crack has the same depth as the pit at the point of transition and initiates at the pit base, has no intrinsic foundation. In fact, novel observations using X-ray tomography of stress-corrosion cracks emerging from pits showed that cracks evolved from the pit predominantly at or near the pit mouth and not at the pit base. Moreover, recent finite element analysis of pits in specimens subjected to different static loads revealed that maximum stress and strain can occur at the pit shoulder and in the proximity to the pit mouth. This study presents numerical predictions of pit evolution from flat metal surface to realistic pit morphologies by using a new technique called peridynamics [2,3]. References [1] R. J. H. Wanhill, R. T. Byrnes, and C. L. Smith, “Stress corrosion cracking (SCC) in aereospace vehicles,” Woodhead Publishing, pp. 608-650, 2011. [2] S. A. Silling, “Reformulation of elasticity theory for discontinuities and long-range forces,” J. Mech. Phys. Solids, vol. 48, pp. 175–209, 2000. [3] D. De Meo, C. Diyaroglu, N. Zhu, E. Oterkus, and M. Amir Siddiq, “Modelling of stress-corrosion cracking by using peridynamics,” Int. J. Hydrogen Energy, vol. 41, pp. 6593–6609, 2016.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Peridynamics for Damage Prediction in Composite Laminates due to Thermo-Oxidation

Author(s): *Selda Oterkus, *University of Strathclyde*; Erdogan Madenci, *University of Arizona*.

Surface oxidation degrades the durability of polymer matrix composites operating at high temperatures due to the presence of strong coupling between the thermal oxidation and structural damage evolution. The thermo-oxidative environment results in growth of the thermo-oxidative layer and changes in material properties. The degradation mainly occurs on the surface layer, and it leads to weight loss and shrinkage of the oxidized layer. Therefore, prediction of long-term durability requires the consideration of both the oxidative changes and damage evolution. The analysis of damage due thermal oxidation is fundamentally multi-physical and multi-scale in nature. Therefore, this study presents the PD modeling of isothermal aging of composite laminates. The oxidation degradation is modeled by coupling chemical and mechanical responses of the material and damage evolution. It incorporates multiple physical phenomena under one computational framework, peridynamics, which directly and fully couples the distinct physics involving mechanics of deformation, diffusion of temperature, oxygen concentration. The effects of material failure/damage is immediately influence local material properties governing the fields of diffusion. The PD theory enables the coupling of different fields such as thermomechanics and hygrothermomechanics [1-7]. References: [1] Oterkus, S., Madenci, E., & Agwai, A. (2014). Fully coupled peridynamic thermomechanics. Journal of the Mechanics and Physics of Solids, 64, 1-23. [2] Oterkus, S., Madenci, E., Oterkus, E., Hwang, Y., Bae, J., & Han, S. (2014, May). Hygro-thermo-mechanical analysis and failure prediction in electronic packages by using peridynamics. In Electronic Components and Technology Conference (ECTC), 2014 IEEE 64th (pp. 973-982). IEEE. [3] Oterkus, E., & Madenci, E. (2012). Peridynamic analysis of fiber-reinforced composite materials. Journal of Mechanics of Materials and Structures, 7(1), 45-84. [4] Madenci, E., & Oterkus, E. (2014). Peridynamic theory and its applications (Vol. 17). New York: Springer. [5] Oterkus, S., & Madenci, E. (2014). Fully coupled thermomechanical analysis of fiber reinforced composites using peridynamics. In 55th AIAA/ASMe/ASCE/AHS/SC Structures, Structural Dynamics, and Materials Conference-SciTech Forum and Exposition 2014. [6] Oterkus, S. (2015). Peridynamics for the solution of multiphysics problems. [7] Oterkus, S., Fox, J., & Madenci, E. (2013, May). Simulation of electro-migration through peridynamics. In Electronic Components and Technology Conference (ECTC), 2013 IEEE 63rd (pp. 1488-1493). IEEE.

14th U.S. National Congress on Computational Mechanics
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Title: A FEAST-Type Algorithm for Operators

Author(s): *Jeffrey Ovall, Jay Gopalakrishnan, *Portland State University*; Luka Grubisic, *University of Zagreb*.

The FEAST algorithm, and other similar algorithms based on rational approximations of the spectral projector, are becoming increasingly popular in the linear algebra community. We present a FEAST-type algorithm for operators on Hilbert spaces, having in mind important differential operators as motivation for the general theory. An error analysis will be provided that incorporates both the error inherent in approximating the spectral projection associated with the given operator by a rational function of the operator, as well as the error arising from the discrete (finite rank) representation of the resolvent of the operator. A realization of the algorithm for differential operators that uses Discontinuous Petrov-Galerkin discretizations, will be described, and its performance demonstrated numerically.

14th U.S. National Congress on Computational Mechanics
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Title: Geometry and Mesh Generation for Representative Volume Elements in Computational Materials Modeling

Author(s): *Steven J. Owen, James W. Foulk , Benjamin Reedlun, Coleman Alleman, Hojun Lim, *Sandia National Laboratories*; Corey Ernst, *Elemental Technologies*.

We propose a new toolkit for generating both unstructured hexahedral and tetrahedral meshes for the analysis of complex composite materials with the finite element method. Computational materials modeling frequently utilizes a simple cuboidal representative volume element (RVE) to characterize complex particle interactions and yield the effective mechanical properties of a medium. A composite material can be represented by a dense Cartesian grid where each cell is assigned a single ID or set of volume fractions that indicate materials contained in each cell. Current computational methods often use a stair-step interface between materials in the structured grid. It has been shown that stair-step material interfaces can often introduce artificial stress concentrations leading to inaccurate predictions of near-field and far-field material behavior. An alternative geometric representation and mesh generation method is presented where smooth, conformal, interfaces are produced for use in a traditional Langrangian FEA code. The proposed toolkit is based upon an interface reconstruction technique known as “primal contouring,” where the vertices of the Eulerian Cartesian grid are modified to conform to an approximated geometric interface extracted from volume fractions. A full boundary representation (B-rep) solid model consisting of a merged set of volumes, surfaces, curves and vertices is extracted from the inter-cell material topology. Curve and surface geometries are constructed as discrete manifolds composed of edges and triangles. Laplacian smoothing combined with optimization-based methods are utilized for smoothing and maintaining suitable geometric interfaces of the composite structures. Tetrahedral meshing of the discrete B-rep that is produced is accomplished using Sandia’s Cubit Geometry and Meshing Toolkit. This provides a geometry-sensitive adaptive tet mesh where an arbitrary mesh size may be specified for a range of mesh resolutions from the same geometric model. Hexahedral meshing is accomplished utilizing the Sculpt tool, a companion application to Cubit, that uses a parallel overlay grid method for generating the all-hex mesh. In this case, the Cartesian cells serve as the basis of the hex mesh while layers of hexes, or “pillows”, are inserted at the grain interfaces. Smoothing and additional pillowing operations are employed to correct for poor quality hexes generated on curves and surfaces. We also propose and demonstrate methods for adaptively refining the hexahedral mesh to better represent geometric features using a conformal two-refinement technique. Inclusion of thin boundary layers to represent interphase layers between materials is also demonstrated where additional controlled pillow layers can be inserted between materials.

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Title: Average-Worst-Case Topology Optimization Using Stochastic Programming and Conditional Value-at-Risk

Author(s): *Geoffrey Oxberry, Cosmin Petra, Mark Stowell, Andrew Barker, Daniel White, Daniel Tortorelli, *LLNL*.

Additive manufacturing has enlarged dramatically the design space in engineering applications by enabling designers to manufacture parts of almost any shape. Deterministic formulations of topology optimization problems assume a fixed number of possible boundary conditions (e.g., load cases in solid mechanics), constant/homogeneous material properties, and no geometric variability. However, these three assumptions are violated in practical experience, and could affect substantially design performance. Stochastic topology optimization formulations attempt to compensate for these violated assumptions. Traditional approaches to formulating stochastic topology optimization problems tend to use linear combinations of the mean and variance (or standard deviation) of a design figure of merit (e.g.,compliance) with respect to a given probability density. However, this choice of mean-variance objective (or constraint) tends to underweight worst-case events in non-normal probability distributions. Borrowing an approach for modeling financial risk, we propose replacing mean-variance expressions with the conditional value-at-risk (CVaR), where the x-CVaR of a random variable is its expected value over the worst x% of cases -- the “average-worst-case". We present a CVaR-based stochastic programming formulation for compliance minimization, and compare its performance with mean-variance formulations. Using results from these case studies and from the stochastic programming literature, we argue the case that CVaR better compensates for worst-case tail events by showing differences in the CVaR of the design figure of merit compared to the CVaR of this figure of merit computed using mean-variance formulations.

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July 17-20, 2017, Montreal, Quebec, Canada

Title: A Practical Method for Automatic Camera Paths Generation in Scientific Visualization Storytelling

Author(s): Anis Benyoub, *École polytechnique de Montréa*; *Benoît Ozell, *École polytechnique de Montréal*.

Camera path planning is a recurrent task in disciplines such as computer vision, animated character motion, and video games. Solutions based on constraint system resolution and system optimization have proven to be efficient ways to build interesting camera paths either in a real environment or a virtual reality scene. However, the task of generating a relevant camera path for exploring 3D scientific data is still a frequently encountered problem. Scientific visualization scenes are at a disadvantage when compared to video games and cinematographic scenes: characters, objects and environments are notions that do not exist. In this work, we introduce a meta-modelisation of scientific scenes using storytelling notions, and we import camera path generation techniques from cinema and video games. We present a complete methodology to automatically create camera paths for scientific results and to easily produce video sequences. Our technique defines a feature as a data behavior that is interesting and worth observing in the numerical results, and we use these features as a basis for camera placement and movement. Some of these features (data behaviors deemed worth looking at) are streamlines and vortices over the velocity vector field; shockwaves as discontinuities in physical properties such as pressure, density, or velocity; and regions containing separation and attachment lines. Given a set of features, our goal is to generate a set of camera paths instead of one single visualization scenario. The camera paths are heuristically generated, resulting in a series of video sequences that the user can choose from. Time varying numerical results require more processing as state tracking, regions of interest, and time coherency are important facets of feature detection. We also enforce slower camera movements in the generated camera paths since quick camera movements can be confusing if the scene content is changing at the same time as the point of view. Our results on various scene samples showed that our methodology is a quick and efficient way for generating multiple scene-relevant camera paths. Even if the method is oriented towards automatic path generation, the scientist can intervene in the generation process at each step (weight setting, initial viewpoint, path building, interpolation, and film editing) in a way to make the final cut fit more his expectations. The scientist's interactions remain intuitive and give him accurate control on the generated scenarios. Producing a final cut to present results becomes a much easier task.

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Title: Multi-Scale Modeling of Fatigue Crack Initiation in Polycrystalline Titanium Alloys

Author(s): *Deniz Ozturk, Somnath Ghosh, *Johns Hopkins University*; Shravan Kotha, *Johns Hopkins University* .

In this work, a recently developed parametrically-homogenized continuum model is used in coupling with micro-mechanical crystal plasticity and crack initiation models to investigate sub-surface dwell fatigue crack initiation in Titanium alloys, through multi-scale simulations accounting for microstructural variability. To develop image-based micromechanical models, microstructural data are obtained from Electron Back-Scattered Diffraction (EBSD) maps and are used to generate statistically-equivalent polycrystalline models. A rate-, size- and temperature-dependent Crystal Plasticity Finite Element (CPFE) model for polycrystalline Titanium alloys is used to compute material deformation as a function of microstructural properties. The CPFE simulations are accelerated using a multi-time scale integration technique to compute local stress and dislocation content over large number of fatigue cycles. An experimentally validated probabilistic model is then used to predict fatigue crack initiation as a function of microstructure and loading conditions. Following a sensitivity study to identify the microstructural properties governing the constitutive response of Ti-alloys, CPFE simulations are performed on polycrystalline models with various microstructural properties and under various loading conditions. The CPFE response data is used to develop a parametrically-homogenized microstructure-sensitive elasto-plastic constitutive model for polycrystalline Ti alloys, which is used for macroscopic simulations. To predict crack initiation in fatigue test specimens of extruded Ti-7%Al, macroscopic 3D models are generated accounting for the spatial variations of the microstructure. Microstructural parameters are first assigned to the model domain by sampling from the EBSD scans. To quantify the spatial variability of the microstructure, auto-correlation functions of crystallographic (0001) axes are calculated from the EBSD scans which are obtained from three orthogonal faces of the extruded material. In an iterative algorithm, the spatial distribution of the microstructural parameters are evolved to match the correlation structure of the 3D specimen. This process adequately generates micro-textured regions in the macroscopic model, which are features known to be detrimental to the dwell fatigue performance of Ti alloys. These microstructural variations are shown to significantly influence the local stress response, which is amplified up to 50% above the applied stress. The local stress-strain histories from the macroscopic fatigue simulations are then imposed as boundary conditions to detailed micromechanical CPFE and crack nucleation simulations, to predict cycles-to-initiation, location and orientation of dwell fatigue cracks initiating from grain boundaries. A phase field fracture model coupled with crystal plasticity is being developed for predictions of crack propagation in polycrystalline Ti.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Validation of Numerical Simulation Results of E-Defense Large Scale Experiment on Soil-Underground Structure Interaction

Author(s): *Mahendra Kumar Pal, Takuzo Yamashita, *NIED, Japan*; Shintaro Ohno, *Kajima Cooperation, Japan*; Atsushi Iizuka, *Kobe University, Japan*.

A systematic analysis of both experimental and numerical study of Soil-Structure-Structure Interaction (SSSI), in a comparative manner with an aim to validate the numerical results of E-Simulator, is presented here. A large-scale soil-underground structure specimen, comprises of two layers of soil-strata, two vertical shafts, two horizontal shield tunnel and one cut-and-cover tunnel interconnecting the shafts, was tested against multiple seismic input waves [1], seeking better understanding of soil-structure interaction. E-simulator [2] is in-house high performance parallel FE package developed at and by E-Défense to reproduce the damage mechanism of buildings and civil structures against seismic loading. A detailed finite element model of test specimen is generated and meshed with solid 3-dimensional linear tetrahedral elements. Interface between soil and structures is ensured by conforming mesh. To simulate elastoplastic behaviour of soil, the exponential contractancy model, introducing sub-loading surface [3] is implemented as a constitutive model for soil. Detailed FEM model of specimen is analyzed using E-Simulator. Time histories of displacement, strain and acceleration response at different locations along vertical shafts and shield tunnels are compared with experiment results along with dynamic behaviors of various components of specimen. A comparative study of profiles of curvature, rotation and displacement along tunnel is also presented. The obtained numerical results are in reasonable agreement with the E-Défense large-scale experiment. A torsional deformation of cut-and-cover tunnel is also reported. Keywords: Soil-Structure-Structure Interaction, Large-scale Shake Table Test, Underground Structures, Validation, E-Simulator, E-Defense. References: [1] Yohsuke Kawamata, Manabu Nakayama, Ikuo Towhata, Susumu Yasuda, “Dynamic behaviour of underground structure in E-Defense shaking experiment”, Soil dynamics and earthquake engineering, 82, pp. 24-39, 2016. [2] Takuzo Yamashita, Muneo Hori, Koichi Kajiwara. “Petascale Computation for Earthquake Engineering”, Computing in Science and Engineering, 13(4), pp. 44-49, 2011. [3] Shintaro Ohno, “Elasto-plastic constitutive models derived from non-linear description of soil contractancy”, Doctoral thesis submitted to Tokyo Institute of Technology Japan, 2006.

14th U.S. National Congress on Computational Mechanics
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Title: A Cut Cell Finite Element Method for Poisson's Equation on Irregular Planar Domains

Author(s): *Sushrut Pande, Panayiotis Papadopoulos, *UC Berkeley*.

This talk presents the development of a cut cell-based finite element method to solve Poisson's equation on structured grids (such as those generated, e.g. from digitized images [1]) in the presence of arbitrarily-shaped boundaries. In present practice, such grids are typically truncated by outright removing elements that fall outside the physical domain, thus leading to stair-step shapes and their (often undesirable) effects on convergence. The present work is motivated by earlier finite-volume technologies [2] and attempts to overcome this challenge by instead solving the differential equation on a Cartesian axis-aligned grid which is neither "rough" nor fitted to the boundary of the physical domain. Rather, the domain is first immersed inside a regular grid and then all elements are classified according to their relative position to the boundary (inside, outside, or partial). The resulting bounding box of the domain is subjected to Dirichlet and Neumann boundary conditions using tractable geometric information from the partial cells. For Dirichlet boundary conditions, the nodes of partial cells lying outside the domain are projected onto boundary points of the domain, where the boundary conditions are strongly enforced pointwise. For Neumann boundary conditions, the weak form of the differential equation is accurately integrated over a locally triangulated approximation of the actual physical domain. The method is tested on a range of planar problems for which analytical solutions are known. For both cases, it is observed that this method attains the same theoretical asymptotic convergence rates as those achieved by unstructured mesh finite element methods. References: [1] M.F. Adams, H.H. Bayraktar, T.M Keaveny and P. Papadopoulos, Ultrascalable Implicit Finite Element Analyses in Solid Mechanics with over Half a Billion Degrees of Freedom, ACM/IEEE Proceedings of SC2004: High Performance Networking and Computing. [2] H. Johansen and P. Colella, A Cartesian Grid Embedded Boundary Method for Poisson's Equation on Irregular Domains, Journal of Computational Physics, 147(1):60-85 (1998).

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Title: Assessment of Soil Inertia Effects in Dynamic Analysis of Piles under Impact Loading

Author(s): Gustavo Pacheco, *Polytechnic University of PR*; Luis Suarez, *University of PR at Mayaguez*; *Miguel Pando, *U of North Carolina at Charlotte*.

It is common practice to analyze single piles under dynamic lateral loads (e.g., seismic or impact) with a relatively simple discrete nonlinear Winkler model. In this popular and simplistic approach the pile is modeled as beam elements and the soil reaction is represented by independent, concentrated nonlinear springs that act normal to the pile longitudinal axis. The literature shows that for dynamic analyses of piles, the soil stiffness and damping properties can be adequately included through lumped springs and dashpots. In contrast any possible soil inertia effects are not considered. Soil inertial effects can be easily introduced in the discrete Winkler-type models through lumped masses that can represent the soil inertia effects. The objective of this presentation is to present a simple model that includes the soil inertial effects in the problem of dynamic laterally loaded single piles. The methodology presented is based on a lumped model consistent with the Winkler proposition that allows investigating the relative importance of soil inertial effects on the dynamic response of single piles. The parameters needed for the proposed discrete model were obtained by approximating the continuous, plane strain model developed by Novak. In the proposed approach, the pile-soil interaction is accounted for by three frequency independent elements: a spring with stiffness ka, a mass ma, and a dashpot with coefficient ca. The spring-mass-dashpot coefficients representing the soil are defined by simple equations. The proposed model shows that soil-inertial effects are negligible for soil profiles with a small to medium soil Poisson's ratio. However, consideration of the soil mass was found to be important for soil deposits with high Poisson's ratios (e.g., undrained loading of saturated soils where $\nu = 0.5$). For the case of saturated soils the inertia contribution due to the soil lumped masses can be of the same order of the pile mass.

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Title: Internal Explosion Simulation of Earth Covered Composite Arch System; the Comparison between MMALE, PBM and CONWEP+GP Methods

Author(s): *Sze Dai Pang, *National University of Singapo*.

In the investigation of dynamic response of earth covered composite arch structure against internal explosion, it was found that the loading is different from the free air explosion. The loading curve is characterized by a high pressure spike termed shock phase, followed by a prolonged gas pressure phase. Multiple peaks of shock pressure are observed due to the reflections and interactions of blast pressures within the structure. The reflections decay over time and the duration of the gas pressure phase depends on the level of venting provided. The structure of interest has two steel doors at both ends, which translates to some degree of venting as the steel doors will be blasted away due to the high pressure generated from internal blast. Finite element model is constructed in LS-Dyna software using three different methods, fully coupled Multi-Material Arbitrary Lagrangian Eulerian (MMALE), fully coupled Particle Blast Method (PBM) and decoupled method of combining gas pressure from MMALE and CONWEP curve (CONWEP+GP). The paper will describe the modelling of the earth covered composite arch structure and the three methods of blast load modelling. The accuracy and efficiency of each method will be compared by measuring the buried composite arch maximum deflection, blast door velocity and computational time.

14th U.S. National Congress on Computational Mechanics
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Title: Through Thickness Reinforcement for Z-Pinned Composites

Author(s): *Mark Pankow, *North Carolina State Universit*.

Interlaminar delamination has been identified as a dominant damage mode for laminated composites subjected to impact. More commonly referred to as barely visible impact damage (BVID), impact can cause major drop in residual stiffness and strength of parts. In order to overcome delamination, through the thickness reinforcement (TTR), such as z-pinning and stitching, have been used frequently and shown substantial improvements in delamination resistance and residual strength of laminated composites. The main objective of this research is to investigate the delamination due to impact and estimate the residual strength of z-pin reinforced composite using finite element analysis. Considering the small size of individual z-pins relative to the size of the laminate, modeling detailed geometric features of z-pins is computationally expensive. By characterizing the effect of z-pin reinforcement through a material model without discretely modeling the z-pin geometry, the impact response of laminated composites can be captured accurately with a reasonable computational expense. A modified cohesive law has been developed to accurately capture the details of pin failure. Pure mode I and mode II properties of z-pin reinforced composites are evaluated using the double cantilever beam (DCB) and the end notch flexure (ENF) tests, respectively. Based on these values, the mixed mode behavior of z-pinned composites is estimated with a detail FE model of individual Z-pin reinforcements. The results from this finite element model are then turned into the effective properties for a modified cohesive law which will be used to model the delamination during impact and compression after impact analysis. For an equivalent model using a tri-linear interface behaviour is implemented using the Abaqus user defined field (VUFIELD) subroutine. This subroutine divides the damage evolution energy in two regions. Based on the user input from experimental results, the effective response transitions from an elastic deformation to a frictional pullout. The equivalent model will also include modification to the simulated mode II and mixed mode response of z-pin reinforcement. The finite element modeling of impact and the compression after impact of an unreinforced composites have been reported earlier. By implementing the material model mentioned above, the existing computational scheme will be enhanced to predict the response of z-pin reinforcement and compared against the experimental results for validation.

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Title: Comparison of Human Brain Finite Element Models to Whole Brain Sonomicrometry Data

Author(s): Ahmed Alshareef, Sebastian Giudice, Jason Forman, *Matthew B. Panzer, *University of Virginia*.

Traumatic Brain Injury (TBI) presents an urgent public health concern. The Center for Disease Control reports that the annual incidence of TBI amongst civilians in the United States is approximately 1.7 million, of which 75% are mild TBI or concussion. Finite element (FE) models of the brain are the gold standard for predicting injury severity and the effectiveness of safety gear in mitigating injury. They use strain-based metrics of brain deformation to predict injury. These models, however, have been developed using limited validation data. The objective of this study was to compare the response of two widely used brain FE models, GHBMC and SIMon, to recent, highly accurate in situ 3D brain motion data. In a previous study, validation data for brain motion was obtained using an array of neutrally dense sonomicrometry crystals that were implanted into the brain tissue of a single cadaveric head specimen. Distance measurements were calculated using speed of sound of the tissue and then trilaterated to quantify the 3D displacement time-history of the crystals within the brain tissue. Four pure rotational impacts, ranging from 20 – 40 rad/s with durations of 30 – 60 ms were applied to the head/brain specimen in the three anatomic planes. Two brain FE models, GHBMC, and SIMon, were used to compare the motion of the crystals and the brain. The motion of nodes was tracked to compare to the validation sonomicrometry data. Three methods were implemented for this validation: 1) using absolute coordinates of the initial crystal position to find the corresponding node, 2) using relative coordinates based on the maximum length, width, and height of the head to find the corresponding node, and 3) using structural scaling to scale the FE model to the cadaveric head. Preliminary results indicated that FE models are not well validated for brain deformation. This is the first study to compare the response of human brain FE models to 3D whole brain motion data acquired from a single specimen with rotations in all three anatomical planes. The response of the model and the experimental data was observed to differ in magnitude and duration of the transient response of the brain, as well as be regionally-dependent. There were some differences between the three validation methods, but none closely matched the experimental data. Future work includes using morphing as an additional validation method and to compare differences in response and correlate them to structural or material properties.

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Title: Multiscale Optimization of Carbon-Nanotube Reinforced Polymer Structures

Author(s): Maria Tavlaki, Odysseas Kokkinos, *Vissarion Papadopoulos, Manolis Papadrakakis, *NTUA*.

Carbon nanotubes belong to a promising class of carbon allotropes, whose high strength and low weight renders them ideal for applications where minimizing the weight of the structure is crucial, such as in aerospace engineering. However, owing to the current paucity of technical expertise and relevant infrastructure, the production of nanotubes, whose diameter is in the range of nanometers, is relatively expensive- therefore optimizing the nanotubes' characteristics when using them as a reinforcing agent can yield significant financial gain. The current work proposes a novel three-level multiscale optimization technique to optimize the orientation and dispersion of nanotubes in benchmark carbon nanotube-polymer structures. At the lowest, atomic level a short portion of the nanotube was modeled using molecular mechanics and subsequently approximated by a series of equivalent beam elements at the next microscopic level. At this level, a Representative Volume Element consisting of a straight nanotube embedded in polymer was analyzed and approximated at the next level using a first-order homogenization technique [1]. Finally, at the macroscopic level, a macroscopic structure was analyzed concurrently with the previous level using a nested solution scheme [2]. One RVE corresponding to a nanotube orientation and diameter was assigned to every Gauss point of the finite elements into which the macroscopic structure is discretized. Using the NSGA-II multi-objective optimization algorithm [3], a set of nanotube angles and diameters was calculated so that the energy for each macroscopic structure is minimized, under the constraint that the mean nanotube volume fraction over the macroscopic structure has to remain constant. Acknowledgement: This work has been supported by the European Research Council Advanced Grant "MASTER – Mastering the computational challenges in numerical modeling and optimum design of CNT reinforced composites" (ERC-2011-ADG_20110209). [1] V. G. Kouznetsova, "Computational homogenization for the multi-scale analysis of multi-phase materials," Technische Universiteit Eindhoven, 2002. [2] F. Feyel, "A multilevel finite element method (FE2) to describe the response of highly non-linear structures using generalized continua," Comput. Methods Appl. Mech. Eng., 192, 3233–3244, 2003. [3] Deb K, Pratap A, Agarwal S, Meyarivan T. "A fast and elitist multi-objective genetic algorithm: NSGAII." IEEE Trans Evol Comput 2002;6(2):

14th U.S. National Congress on Computational Mechanics
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Title: Adaptive Optimization of the Topology of Lattices

Author(s): *Antonin Paquette-Rufiange, Serge Prudhomme, Marc Laforest, Augustin Schmidt, *École Polytechnique Montréal*.

Lattice structures represent one of the most interesting and innovative capabilities that additive manufacturing now offers for the design and fabrication of mechanical parts. These structures present the advantages of being lightweight while satisfying the design requirements. These two characteristics combined now allow the development of new solutions in the domain of biomechanics, aeronautics and automotive industries. For the former, the creation of lattice increase the biocompatibility of prosthesis, while for the latter, the decrease of mass leads to significant economies in fuel consumption. The design of a lattice is a challenging problem because there is so much variability in how to fill a given geometry with trusses. Nowadays, lattices are designed in a conformal way, meaning that some predefined cell is repeated inside a particular piece. However, this simple choice for the design of a lattice is not necessarily the best one regarding the specific application for which the lattice is dedicated. Also, this choice certainly does not exploit the full capabilities of additive manufacturing. The design problem is a topological optimization problem. Several techniques, such as the Solid Isotropic Material Penalization, are used in industry to address this problem. Unfortunately, these methods are constructed around homogenization techniques that do not represent the full range of physical and geometrical parameters present in unstructured lattices. The present work develops a consistent framework for the optimization of lattice structures that could be applied to a wide range of physical models. The framework combines the adaptive optimization of the lattice with the adaptation of the physical model. The proposed method consists of optimizing, with respect to an engineering objective (mass, energy of deformation) and some parameters (the nodes linking the trusses, the area of these trusses) of an initially coarse lattice. In order to reduce the size of the problem, we describe the mechanical properties of the lattice with unidimensional models such as Euler-Bernoulli and Timoshenko beam. After an optimal solution has been found, we add new trusses in the relevant regions and we repeat the optimization process. For this presentation, we describe the theoretical framework of our adaptive method and some numerical examples.

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Title: Coupling Strategies for X/G-FEM Simulation of Hydraulic Fracture

Author(s): *Matin Parchei-Esfahani, Robert Gracie, *University of Waterloo*.

In simulations of hydraulically induced fractures, numerical stability issues normally arise when the coupled hydro-mechanical problem is solved sequentially. Such issues are usually more intense when simulating hydraulic fracture propagation in low-permeability formations as dissipation of energy through fluid leak-off is prevented. Instability is especially evident when flux boundary condition is imposed at the point of injection. In the simulation of fluid flow in porous media, application of an undrained operator splitting technique results in a stable procedure while the drained split exhibits stability issues [1,2]. Available coupling techniques for simulation of hydraulic fractures in low-permeability rocks are mainly comparable with the drained split in porous media, and therefore exhibit numerical instability. In analogy with porous media, a coupling strategy based on the undrained split is expected to reduce the aforementioned stability issues when simulation of hydraulic fractures in low permeability rock is concerned. We present a new locally mass-conservative sequential coupling strategy for hydro-mechanically coupled problems in which the fluid equation is solved first. The proposed strategy is analogous to the undrained split used in poromechanics. The study focuses on propagation of hydraulic fractures in low-permeability rocks where stability issues are expected to be more intense. Comparison of the results for the existing sequential coupling strategies with the results of the new coupling strategy shows that the latter presents a stable procedure with faster convergence. The proposed strategy is stable for problems with either flux or pressure boundary conditions at the point of injection. References: [1] Kim, J., Tchelepi, H. A., and Juanes, R. (2011). Stability and convergence of sequential methods for coupled flow and geomechanics: Drained and undrained splits. Computer Methods in Applied Mechanics and Engineering, 200(23-24), 2094-2116. [2] Mikeli■, A., and Wheeler, M. F. (2013). Convergence of iterative coupling for coupled flow and geomechanics. Computational Geosciences, 17(3), 455-461.

14th U.S. National Congress on Computational Mechanics
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Title: Statistical Mechanics-Based Closures for Galerkin ROMs

Author(s): *Eric Parish, Karthik Duraisamy, *Univ of Michigan*.

The use of reduced-order modeling (ROM) techniques in problems that lack a clear separation of scales is hampered by our inability to derive consistent closures. Adhoc closures derived using phenomenological assumptions can mispredict the transfer of information across scales. In this work, we use the Mori-Zwanzig (M-Z) formalism to represent the impact of the unresolved modes on the resolved modes. The M-Z approach is rooted in non-equilibrium statistical mechanics and offers a mathematically consistent procedure to derive closure models. In the M-Z approach, the unclosed terms can be formally represented as a memory integral, which is, in general intractable for non-linear problems. We will present a technique to model the memory kernel and demonstrate applications in ROMs of turbulent flow.

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Title: Molecular Dynamics Analysis of DNA-Micelle Complex and Its Electrophoretic Transport for Drug Delivery System

Author(s): *Jae Hyun Park, *Gyeongsang National University*; Narayana Aluru, *University of Illinois at Urbana-Champaign*.

Micelles have been popularly used as the vehicles in diverse drug delivery systems for the last two decades. They encapsulate various medical objects such as low molecular weight anticancer drugs, contrast/imaging agents, proteins, plasmid DNA, antisense DNA, and more recently short interfering RNA (siRNA) and those loaded-micelles are delivered to the target area in living system. In the present study, we propose an efficient transport method of micelle with DNA using extensive all-atom molecular dynamics (MD) simulations. For the systematic approach, we first investigate the aggregation of micelles without DNA. Each micelle is trying to be apart as much as possible from the others, and thus the micelles form a stable aggregate overall without noticeable diffusional motion. However, when a single-stranded DNA (ssDNA) is included at the center of micelle groups, the micelles are gathered together around the DNA and a micelle-DNA complex is formed. Some micelles are bound with the ends of DNA first and subsequently the other micelles move to the DNA to fill some empty part of DNA. Although the micelles prefer to be combined with the DNA, due to the geometric hindrance between micelles there exists an optimized number of micelles attached to DNA, which is related with the length of DNA. Then, an electric field is applied to the DNA-micelle complex formed to present its electrophoretic motion, which is not possible for pure micelle aggregate. The atomic configuration in the complex is optimized again due to electric field during the electrophoretic motion. Comprehensive molecule-level analyses about the DNA-micelle complex and its electrophoretic movement will be presented at the conference with focus on the quantification of participating interactions.

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Title: Frictional-Contact Model Coupled with the Traction-Separation Relationship of the Cohesive Zone Model

Author(s): *Kyoungsoo Park, Hyunil Baek, *Yonsei University*.

A cohesive frictional contact model is proposed to investigate nonlinear fracture behaviors under compression. Friction is approximated by using the Lagrange multiplier method in conjunction with the Coulomb frictional model, which accounts for stick-slip behaviors. The normal contact force is estimated by employing the penalty method and/or the Lagrange multiplier method. The Park-Paulino-Roesler (PPR) cohesive model is utilized to characterize the cohesive constitutive relationship, and cohesive surface elements are adaptively inserted to interfaces of bulk elements. To verify and validate the proposed frictional-contact model for the cohesive zone model, three computational examples are employed: bar impact test, dynamic earthquake rupture, and masonry wallettes shear test.

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Title: A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics

Author(s): Payton Lindsay, *Purdue University*; *Michael Parks, *Sandia National Laboratories*.

Peridynamics is a nonlocal reformulation of continuum mechanics that is suitable for representing deformations with discontinuities, see [1, 2] and the references therein. We extend the peridynamic formulation to allow the use of multiple time steps within a single problem domain by decomposing that domain into a number of smaller subdomains, where the critical regions of interest are solved using a small time step and the rest of the problem domain is solved using a larger time step. We explore the numerical properties and computational cost of the proposed approach, and demonstrate through numerical examples that a multi-time-step discretization of peridynamics can be solved much faster than a uniform time step discretization, and without adversely affecting the accuracy of the computed solution [3]. [1] S. A. Silling, “Reformulation of elasticity theory for discontinuities and long-range forces”, J. Mech. Phys. Solids, 48 175–209 (2000). [2] S. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, “Peridynamic states and constitutive modeling”, J. Elasticity, 88, 151–184 (2007). [3] P. Lindsay, M.L. Parks, and A. Prakash, “Enabling fast, stable and accurate peridynamics computations using multi-time-step integration”, Comput. Methods Appl. Mech. Engrg., 306, pp. 382-405, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: Finite-Element Simulation and Optimal Control of Free-Surface Problems

Author(s): *Nicola Parolini, Ivan Fumagalli, Mattia Tamellini, Marco Verani, *Politecnico di Milano*.

We present some recent results on the simulation and optimal control of free-surface problems emerging in different industrial applications, such as ink-jet printing and metal foam production. In ink-jet printing, capillary forces play an important role in the evolution of the free-surface and the numerical approximation requires special care to treat, e.g., the dynamics of the contact angle at the triple point. For the simulation of this kind of free-boundary problem, a numerical model based on the Arbitrary Eulerian Lagrangian (ALE) formulation is employed both in the solution of the direct and inverse problem. The latter aiming at controlling the position of the free-surface. In application such as metal foam production, it is important to be able to deal with complex free-surface geometries and large interface deformations. Moreover, in some operating conditions, it is useful to account for compressibility of the gaseous phase. In this case, an Eulerian approach based on the Level Set method has been preferred. A finite-element solver for incompressible-incompressible and compressible-incompressible free-surface flows is presented. For the fully incompressible case a standard finite-element Level Set solver is considered, while for the compressible-incompressible case a finite-element recast of the model proposed in \cite{LeMaitre} is considered. The direct solver is then employed to tackle an optimal control problem aiming at driving the free-surface interface towards a desired location by controlling a boundary value of the velocity.

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Title: Finite Element Methods for Accurate, Large-Scale Quantum Mechanical Materials Calculations: From Classical to Enriched to Discontinuous

Author(s): *John Pask, *LLNL*.

We discuss recent developments in finite-element (FE) based methods for the solution of the Kohn-Sham equations that have made possible larger, more realistic calculations than possible heretofore by current state-of-the-art planewave (PW) based methods. We begin with classical FE based approaches, demonstrating optimal convergence rates and micro-Hartree agreement with established PW based methods. We then discuss recent partition-of-unity enriched FE (PUFE) methods, which build known atomic physics into the basis while retaining strict locality and systematic improvability. By incorporating known physics, these bases can achieve the required accuracies with an order of magnitude fewer degrees of freedom (DOF) than required by traditional PW based methods. However, with such enrichment comes more costly quadrature, non-orthogonality, and some degree of ill-conditioning. We discuss two directions we are currently pursuing to address these issues while retaining strict locality and systematic improvability: Discontinuous Galerkin (DG) and Particle Partition of Unity (PPUM) methods. We conclude with recent results for quantum molecular dynamics of general metallic and solid-liquid interface systems of 4,000 atoms and more, and discuss issues to be addressed to get to 10,000 atoms and more.

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Title: Multi-Material Continuum Topology Optimization: An Elegant Formulation and Update Scheme

Author(s): *Glaucio Paulino, *Georgia Institute of Technolog*; Emily Daniels, *Georgia Institute of Technology*; Miguel Aguilo, *SANDIA National Laboratory*.

A framework is presented for multi-material compliance minimization in the context of continuum based topology optimization. We adopt the common approach of finding an optimal shape by solving a series of explicit convex (linear) approximations to the volume constrained compliance minimization problem. The dual objective associated with the linearized subproblems is a separable function of the Lagrange multipliers and thus, the update of each design variable is dependent only on the Lagrange multiplier of its associated volume constraint, which is a feature especially suited for large-scale parallel computing. As a result, the so-called ZPR (Zhang-Paulino-Ramos) update scheme can applied in series or in parallel for each volume constraint, and can be leveraged to obtain a unique solution. The key ideas presented herein are demonstrated through representative examples in 2D and 3D.

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Title: Phase-Field Modeling of Surfactant-Driven Fracture in Particulate Rafts

Author(s): *Christian Peco, Yingjie Liu, Carter Rhea, John Dolbow, *Duke University*; Wei Chen, Mahesh Bandi, Eliot Fried, *OIST*.

Hydrophobic particles at a liquid-air interface tend to aggregate and form a monolayer, known as a particulate raft. These particles, otherwise non-cohesive, deform the liquid surface and interact through capillary bridges, enabling the monolayer to withstand tensile and shear deformations. The study of particulate monolayers is of great interest to scientists and engineers due to their potential for stabilizing liquid drops and emulsions via jamming. Experiments show that when a certain particle density is achieved, the raft can be characterized as a two-dimensional elastic solid, the properties of which depend on the liquid layer's surface tension. Consequently, a practical way to further study particle rafts is through the introduction of a controlled quantity of surfactant into the system. Injected at a particular point, the surfactant decreases the surface tension and generates a front, fracturing the monolayer. The crack features observed in particulate rafts are reminiscent of those in traditional media, but with significant differences. Traditionally, these features have been attributed to the initial particle distribution of the monolayer. However, while secondary features (e.g., abrupt changes of direction and crack starting points) may indeed depend on density variations, the general features, such as the number of branches, should arise from more fundamental physical considerations. The goal of this work is to determine the critical physics underlying the surfactant-driven fracture of particulate rafts. We propose a continuum approach based on a phase-field model to describe the damaged zones in the system. In the model, the fracture evolves as a result of the interplay between the pressure exerted by the surfactant and the elastic response of the monolayer. We model the monolayer behavior, accounting for the fracture toughness, the solid rigid nature of the particles, and their initial distribution. The pressure is proportional to the surface tension difference between the surfactant and the liquid layer. A comparison between the experimental observations and the numerical results indicates a qualitative match in both the fracture patterns and temporal scaling of the process. We explore the influence of particle distribution on secondary features (e.g., crack bending). Importantly, we find a dimensionless parameter that characterizes the number of cracks in the final configuration, separating different fracture regimes. We support our findings with new experimental results that confirm the trends inferred from the simulations.

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Title: Scale Analysis of Damage Evolution in Incipient Spall under Plate Impact

Author(s): *xiaoyang pei, shi chen, hui peng, *Institute of Fluid Physics*.

Damage properties of ultrapure copper in plate-impact spall experiments are investigated by means of a wavelet-based multiresolution analysis (MRA) of recovered samples. The one-dimensional (1D) MRA provided detailed information to the averaged void size distribution along the shock-loading direction, and indicate the evolution of spall zone can be divided into fast localization process and slow localization process. The two-dimensional (2D) MRA indicate that the evolution of scale of voids that have important role in the damage state. The characters of the nucleation, growth and coalescence of distributed voids are analysised by field induced percolation and random percolation.

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Title: Implicit Level Set Algorithms for Modeling Multiscale and Turbulent Effects in Hydraulic Fracture Propagation

Author(s): *Anthony Peirce, *University of British Columbia*; Egor Dontsov, *University of Houston*.

A detailed asymptotic analysis of the near-tip behavior of a propagating hydraulic fracture demonstrates that, close to the tip, the fully coupled problem reduces to the solution of a steadily propagating semi-infinite fracture in a state of plane strain. The solution to this simpler problem unmasks the multi-scale nature of the solution that governs both the local behavior of the fracture opening and fluid pressure as well as the location of the fracture's free boundary. In this talk we will describe an implicit level set algorithm (ILSA) that is suitable for exploiting this asymptotic solution to capture multiscale behavior in planar hydraulic fractures propagating in three dimensional elastic media. Because it is able to capture the detailed asymptotic behavior in a weak sense, the ILSA scheme is able to represent the required multi-scale behavior on a relatively coarse rectangular mesh. This is achieved by using the local front velocity to determine the near-tip fracture width solution at all tip elements defined to be those elements that are intersected by the fracture front. Finer-scale behavior is captured in a weak sense by integrating the universal asymptotic solution for the fracture width over the partially filled tip elements and using these integrals to set the average values of the widths there. The ILSA solution shows good agreement with reference solutions comprising a radial fracture that transitions between viscosity, toughness and leak-off dominated propagation regimes. The ILSA scheme is also used to model blade-like hydraulic fractures that break through stress barriers. In this case, different parts of the fracture-free-boundary can be propagating in different regimes. In addition, the effect of turbulent flow is incorporated by replacing the friction factor for laminar flow with the one that is able to capture the laminar-to-turbulent flow transition. The laminar asymptotic solution is still used within the ILSA framework since the Reynolds number is sufficiently small near the tip that the flow is laminar. We also provide examples in which this methodology is used to model multiple hydraulic fractures that propagate simultaneously in parallel planes.

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Title: How Many Ways are there to Subdivide a Hexahedron in Tetrahedra?

Author(s): *Jeanne Pellerin, Jean-Francois Remacle, Amaury Johnen, *UCL, Belgium*.

Indirect hex-dominant meshing methods rely on the recombination of the elements of a tetrahedral mesh into hexahedra. Before combining tetrahedra into hexahedra, we should be able to enumerate the different subdivision patterns of a hex into tetrahedra. We will show that when distorted, however valid, hexes are accounted for, the number of possible subdivision patterns is much larger than previously thought [1]. We will present an algorithm that does not rely on any predefined pattern and is able to discover a whole range of new hex subdivision patterns.
[1] Sokolov D, Ray N, Untereiner L, Levy B. Hexahedral-Dominant Meshing. ACM Transactions on Graphics. 2016; 35(5):1–23.

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Title: A Robust Lagrange-Projection Splitting Scheme for Compressible Multiphase Flows with Viscous and Heat Conduction Effects: Application to the Melting Process

Author(s): *Simon Peluchon, Gérard Gallice, *CEA-CESTA*; Luc Mieussens, *Univ. Bordeaux & INRIA*.

The present work takes place in the context of the atmospheric re-entry problem. This study can concern re-entry vehicles globally or partially made of metallic components, like space debris for instance. During the re-entry phase, a solid undergoes a heating due to the friction of atmospheric gases. Conversion of kinetic energy to thermal energy leads to a sudden increase of the temperature of the object. This rise drives to a physical-chemical degradation of the thermal protective system, and to a boundary recession. There are two main causes of the solid ablation during the re-entry phase: the fusion of the metallic part, which creates a liquid phase into the gas flow, and the sublimation process leading to an injection of gas into the atmosphere. In order to simulate these phenomena, a compressible multiphase flow model needs to be coupled with a heat equation inside the solid. In the present work, our solvers are based on the Finite Volume Method to solve compressible Navier-Stokes and heat equations. A splitting strategy to compute compressible two-phase flows using the five-equation model with viscous and heat conduction effects is presented. The main idea of the splitting is to separate the acoustic and dissipative phenomena from the transport one. The acoustic and dissipative step is solved in a non-conservative form using a scheme based on an approximate Riemann solver. Since the acoustic time step induced by the fast sound velocity is very restrictive, an implicit treatment of this step is performed. For the transport step driven by the slow material waves, an explicit scheme is used. The overall scheme resulting from this splitting operator strategy is very robust, conservative, and preserves contact discontinuities. The boundary interface condition between the solid and the multiphase flow is enforced by mass and energy balances at the wall. The melting front is tracked explicitly using an ALE formulation of the equations. The robustness of the approach is demonstrated through numerical simulations involving large density ratios. The computation of the melting process with a two-phase flow is also presented.

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Title: A Novel Fast Model Predictive Control Method for Large-Scale Stochastic Dynamic Systems

Author(s): *Haijun Peng, Sheng Zhang, Zhigang Wu, *Dalian University of Technolog*.

To reduce the unwanted vibrations and to lessen the probability of structural failures, especially for large-scale stochastic dynamic systems, a novel fast model predictive control (NFMPC) method is presented in this paper. Based on the linear stochastic dynamic equation, a novel explicit expression form of Newmark-β method is first derived, from which the future states can be easily predicted without the computation of the matrix exponential. By applying this explicit expression form into the standard model predictive control (MPC) method, the NFMPC method is developed. Based on the explicit expression form, the optimal control input can be computed by two off-line transient analyses and one on-line transient analysis at every sampling instant on the structure. For no computation of matrix exponential, the off-line computation efficiency of NFMPC is several orders of magnitude higher than that of MPC. And the small amount of on-line computation guarantees the on-line computation efficiency. Furthermore, the use of the Newmark-β method also guarantees the computation accuracy. At last, several typical numerical examples are carried out to verify the validity and high efficiency of NFMPC by the comparison with MPC.

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Title: Hydrogen Assisted Cracking in HCP-Zirconium: a Quasi-Continuum Density Functional Theory (QCDFT) Study

Author(s): *Qing Peng, *University of Michigan*.

The hydrogen assisted cracking is a crucial factor attributing to materials failure. Hydrogen embrittlement in HCP-Zirconium becomes a very important and emergent safety issue which is of interest to academia, industry and policy makers. The hydride formation, diffusion and embrittlement in zircolay will impact dramatically on the development of advanced nuclear energy systems, the life time extension of the current nuclear fleet and dry storage of spent nuclear fuel. Quasi-Continuum Density Functional Theory (QCDFT) is a powerful concurrent multiscale method based entirely on density functional theory (DFT) and allows quantum simulations of materials properties of a large system with billions of atoms. Using QCDFT modeling, we found that the presents of hydrogen at the cracktip of zirconium, both on crack surface and in-bulk, will form zirconium hydrides and embrittle the system. The concentration of hydrogen and orientation of crack plays important roles in such embrittlement. The mechanism of hydrogen embrittlement under various loading conditions will be discussed.

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Title: Preconditioners for the Virtual Element Method: FETI-DP and BDDC

Author(s): Silvia Bertoluzza, *Micol Pennacchio, Daniele Prada, *IMATI-CNR, Pavia, Italy*.

The Virtual Element Method [1] is a quite recent method designed to easily handle meshes consisting of very general shaped polygonal or polyhedral elements. It allows the construction of high regularity approximation spaces which can be described in terms of quite simple degrees of freedom. The method has important features that make it very interesting and competitive: as far as accuracy and stability of the resulting numerical schemes are concerned and simplicity in implementation. However, to ensure that the Virtual Element Method can achieve its full potential, it is also necessary to deal with the efficient solution of the resulting linear system, and, in particular, to provide good preconditioners. In view of a possible parallel implementation of the method we choose here to consider a Domain Decomposition approach [2]. In particular, we focus on two preconditioning techniques which are, nowadays, considered as the most efficient: FETI-DP and BDDC. We prove polylogarithmic condition number bounds, independent of the number of subdomains, the mesh size, and jumps in the diffusion coefficients. We support the theoretical result with numerical tests. [1] L. Beirao da Veiga, F. Brezzi, L.D. Marini, A. Russo: The hitchhiker guide to the Virtual Element Method, Math. Models Methods Appl. Sci., Vol. 24, 1541-1573, (2014). [2] A. Toselli, O. Widlund: Domain Decomposition Methods - Algo- rithms and Theory. Springer Series in Computational Mathematics volume 34, 2005.

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Title: Efficient Parameter Estimation via Multi-Fidelity Bayesian Optimization

Author(s): *Paris Perdikaris, *MIT*; George em Karniadakis, *Brown University*.

We present a computational framework for model inversion using the enabling concepts of multi-fidelity modeling and Bayesian optimization. The proposed methodology targets the accurate construction of response surfaces in parameter space, and the efficient pursuit to identify global optima while keeping the number of expensive function evaluations at a minimum. In particular, we train families of correlated surrogates on available data using Gaussian processes and auto-regressive stochastic schemes. The resulting predictive posterior distribution is used to design an effective adaptive sampling procedure that utilizes the posterior variance estimates to balance the exploration/exploitation trade-off in parameter space. This is a key enabler for practical computations under limited budgets, as demonstrated on a multi-physics problem involving the calibration of boundary conditions in blood flow simulations using three- and one-dimensional flow solvers.

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Title: The DPG Method for High Frequency Time-Harmonic Wave Propagation Problems

Author(s): *Socratis Petrides, Leszek Demkowicz, *ICES, UT Austin*.

In this talk, we outline the most important properties of the Discontinuous Petrov-Galerkin (DPG) method, for the solution of high-frequency wave propagation problems. The DPG method guarantees discrete stability, even in the pre-asymptotic region, and it comes with a built-in local error indicator. This allows for automatic hp-adaptivity, starting from very coarse meshes. In the first part of the talk, we demonstrate these attractive features of the DPG method, by simulating a high frequency Gaussian beam in two space dimension, scattering by a resonating cavity. We start the simulation with a very coarse mesh that captures the geometry, and perform successive hp-adaptive refinements. Our results show that the method avoids unnecessary computations in areas of the domain where the wave doesn't exist, i.e, the mesh is built along with the solution. In the second part of the talk, we present a new iterative solution scheme, for the solution of the DPG system. The need for iterative solvers, comes from the fact that the problem has to be solve several times throughout the adaptive procedure. Employing a direct solver, at every adaptive step is far from optimal and unnecessary. The adaptive refinements can be driven by a partially converged solution, by employing an iterative solver. Being a minimum residual method, DPG always delivers a Hermitian positive definite stiffness matrix. Thus, the Conjugate Gradient (CG) method is the best candidate, provided that it is combined with an effective preconditioner. We introduce such a preconditioner, which exploits information form previous meshes. This new solver is integrated with in the DPG adaptive procedure, by borrowing ideas of the two grid solver technology. We apply our solver for the solution of the acoustics problem in two space dimension. Our results show convergence in terms of iterations at a rate independent of the mesh and the wavenumber.

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Title: TrussQC: Modeling the Fracture of Coarse-Grained Truss Lattices Using the Quasicontinuum Method

Author(s): *Greg Phlipot, Dennis Kochmann, *Caltech*.

The quasicontinuum (QC) method is a powerful multiscale modeling tool originally designed to significantly reduce the computational expense of large atomic lattice simulations. More recently, the QC method was extended to model the nonlinear response of truss lattices by replacing nonlocal atomic potentials with nearest-neighbor bar or beam potentials. The QC method in this talk uses corotational bars and beams as inter-lattice-site connections and an optimized summation rule to approximate the total energy of the system through a weighted sum of sample lattice members. We present results obtained using this QC method, modeling the nonlinear inelastic response of large two- and three-dimensional lattices. In particular, we study brittle and ductile fracture of multiple lattice architectures. Adaptive mesh refinement is used to maintain full resolution along the propagating crack tip, while degrees of freedom in coarse regions are linearly interpolated from representative lattice sites to reduce computational expense.

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Title: Methodology for Generating Hexahedral Finite Element Meshes of Patient-Specific Cartilage Using Image Data from the Osteoarthritis Initiative

Author(s): Borja Rodríguez vila, *Universidad Politécnica de Madrid*; *David Pierce, *University of Connecticut*.

We propose a specific, fully automated methodology for hexahedral meshing of patient-specific geometric structures of the human knee obtained from Magnetic Resonance Images (MRI), i.e. femoral cartilage, tibial plateau and menisci. Osteoarthritis (OA) is a debilitating joint disease that afflicts nearly 20% of people in the US, costing more than $185.5 billion a year (2007) [1]. Mechanical stresses play a key role in the destructive evolution of OA [2]. Only computational models can estimate intra-tissue stresses in human joints because the required in vivo experiments are impossible or unsafe. Finite element (FE) models are a well-established means to estimate stress distributions at the joint scale. Furthermore, we can access large cohort databases of MR Images on the progression of OA, e.g. the NIH-funded Osteoarthritis Initiative (OAI) [3]. Hexahedral FE meshes are preferred over (more easily generated) tetrahedral meshes for a wide range of applications. Unfortunately, building computational meshes from hexahedra is far more restrictive, and a fully automatic approach for generating hexahedral meshes of arbitrary geometries has not yet been achieved. Our methodology uses the minimum bounding box of each cartilage structure to perform customized sweeping algorithms while minimizing the use of collapsed elements. We first label anatomical structures of the knee by manually segmenting sagittal slices of the fat-suppressed 3D dual-echo in steady state. Next we: (1) generate a low-element-density model with a custom sweeping algorithm which takes into account the structure's geometry, (2) apply Laplacian smoothing, (3) refine the model by subdividing hexahedra, (4) expand the model to fit the original (triangular surface) segmentation, (5) smooth the model to eliminate sharp borders, and (6) optimize element quality. Using baseline MRIs from six patients in the OAI database we manually segmented the cartilages and menisci, reconstructed and smoothed them in 3-D, and individually meshed them with hexahedral FEs. In all cases our methodology obtains the patient-specific meshes of interest from the segmented triangular surfaces in less than four minutes (MATLAB implementation on a common PC). Scaled Jacobian values within the meshes range from 0.5 to 1, where ~90% of the elements have values >0.8, and only 1.2% have values from 0.5 to 0.6. Root-mean-square error between hexahedral meshes and surface segmentations is <0.5 mm in all cases. [1] Lawrence, RC et al., Arthritis Rheum, 58:26-35, 2008. [2] Loeser, RF et al., Arthritis Rheum, 64:1697-1707, 2012. [3] Nevitt, M et al., The OAI: Protocol for the Cohort Study, 2006.

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Title: Simple Finite Elements for Geometrically-Exact Bernoulli-Euler Beams and Kirchhoff-Love Shells

Author(s): Sascha Maassen, Nils Viebahn, Jörg Schröder, *Universität Duisburg-Essen*; *Paulo Pimenta, *University of São Paulo*.

Abstract The first objective of this work is to present a fully nonlinear Bernoulli-Euler beam formulation and Kirchhoff-Love shell formulation. The geometrically exact beam formulation is now constrained to obey the Bernoulli-Euler assumption, i.e. the beam is assumed to be shear-rigid. Similarly, the geometrically exact shell formulation is now constrained to obey the Kirchhoff-Love assumption, i.e. the shell is assumed to be shear-rigid. Our approach defines energetically conjugated generalized cross section stress and strains. Besides their practical importance, cross section quantities make easy the derivation of equilibrium equations, as well as the achievement of the corresponding tangent bilinear form, which is always symmetric for hyper-elastic materials and conservative loadings, even far from an equilibrium state. A straight reference configuration and a plane reference configuration are assumed for the beam and shell, respectively. Initially curved elements can then be regarded as a stress-free deformation from this configuration. This approach was already employed for rods and shells in [4,8]. It precludes the use of convective non-Cartesian coordinate systems and other complicate entities like Christoffel symbols and fundamental forms. It simplifies as well the comprehension of tensor quantities, since only components on orthogonal systems are employed. A special definition of rotation is introduced in order to describe the beam torsion that allows easy connections between elements. Two astonishingly simple finite elements for beams and shells are derived, that accomplish the C1-continuity for the displacement field. The work is illustrated by several numerical examples. References 1. Pimenta P. M. and Yojo T., “Geometrically-exact analysis of spatial frames”, Applied Mechanics Reviews, ASME, New York, v.46, 11, 118-128, 1993. 2. E.M.B. Campello, P.M. Pimenta and P. Wriggers, “A triangular finite shell element based on a fully nonlinear shell formulation”, Computational Mechanics, 31 (6), 505-518, 2003. 3. Viebahn, N., Pimenta, P.M. & Schroeder, J., “A simple triangular finite element for nonlinear thin shells - Statics, Dynamics and anisotropy”, Computational Mechanics, online, 2016.

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Title: Recent Advances in the Full Field Modeling of Recrystallization and Grain Growth Using the Level Set Approach

Author(s): *Daniel Pino Muñoz, Marc Bernacki, Nathalie Bozzolo, Thomas Toulorge, Charbel Moussa, Ludovic Maire, Julien Fausty, *PSL - Mines Paristech - CEMEF*.

Digital materials have been progressively taking their place in R&D departments of many industries around the world. The challenge is huge: We want to be able to design a material for a given application while limiting the amount of actual material testing in the laboratory. Within this context we have been working in tight collaboration with industrial partners in order to be able to predict microstructural evolutions of metallic material due to recrystallization and grain growth phenomena. Recently, an original full field model using the level set method in a finite element framework has been introduced in order to simulate in 2D or 3D large scale grain growth and recrystallization problems at the mesoscopic scale. The main idea is to simulate, at the mesoscopic scale, the underlying physical phenomena responsible of the microstructural evolution. This approach allows to deal with an important number of microstructure characteristics (dislocation density, second phase particles, high anisotropy of boundary energy...). In order to achieve such simulations in an efficient way, many numerical methods have to be deployed. In this talk a summary of the latest numerical features implemented within the context of microstructure evolution modeling will be presented. Some examples of applications, including static and dynamic recrystallization, grain growth and zener pinning will be discussed. [1] Maire, Ludovic, et al. "Improvement of 3D mean field models for capillarity-driven grain growth based on full field simulations." Journal of Materials Science 51.24 (2016): 10970-10981. [2] Shakoor, Modesar, et al. "An efficient and parallel level set reinitialization method–Application to micromechanics and microstructural evolutions." Applied Mathematical Modelling 39.23 (2015): 7291-7302. [3] Shakoor, Modesar, Marc Bernacki, and Pierre-Olivier Bouchard. "A new body-fitted immersed volume method for the modeling of ductile fracture at the microscale: Analysis of void clusters and stress state effects on coalescence." Engineering Fracture Mechanics 147 (2015): 398-417.

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Title: Simulation of a Proposed Fluid-Structure Interaction Validation Case

Author(s): *Jonathan Pitt, *Penn State University*.

A new validation test case for low-frequency, large amplitude deformation Fluid-Structure Interaction (FSI) codes is proposed, and simulations of the experiment are presented. This validation case extends previous benchmarks in the literature, by providing high Reynolds number, turbulent, three-dimensional experimental and computational data for FSI algorithms and solution methods comparison. The proposed case consists of a flexible flag attached to a vertically mounted square rod immersed in fully developed pipe flow. This flow is created in the test section of Penn State's twelve-inch water tunnel loop facility. As the flow passes over the square rod, vortices are generated which subsequently excite the flag and cause it to oscillate. The deformation of the flag is the key metric used for experiment-simulation comparison, similar to the two-dimensional laminar computational benchmark of Turek and Hron [1]. A high-resolution simulation of the proposed experiment is performed using an FSI solver previously developed at Penn State [2]. This solver implements a partitioned, overset grid enabled ALE-based method for the solution of tightly coupled FSI problems. In particular, overset meshes are attached to the immersed deformable structure, and permitted to move independently of the static background mesh. The overset grid capability is the enabling technology to allow large deformation of body fitted meshes, required to capture the turbulent boundary phenomena, without the need to re-mesh or distort the grid beyond usability. This approach also allows for simplified meshing of complex geometries, and a reduced domain size for mesh motion calculations, providing for significant reductions in computational cost. Comparison of computational results to experimental measurements are presented. [1] S. Turek and J. Hron. "Proposal of Numerical Benchmarking of Fluid-Structure Interction Between and Elastic Object and Laminar Incompressible Flow", Fluid-Structure Interaction, Vol. 53, pp. 371–385, 2006. [2] S. T. Miller, R. L. Campbell, C. W. Elsworth, J. S. Pitt, and D. A. Boger. "An Overset Grid Method for Fluid-Structure Interaction", World Journal of Mechanics, Vol. 4, No. 7, pp. 217–237, 2014.

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Title: Selective Frequency Damping Algorithm for Steady Flow Convergence Acceleration

Author(s): *Frédéric Plante, Éric Laurendeau, *Polytechnique Montréal*.

This paper presents the use of the Selective Frequency Damping (SFD) algorithm as an acceleration technique for the computation of the Euler and Navier-Stokes equations. The SFD method is implemented in a segregated way [1] in Polytechnique Montreal's in-house CFD software, NSCODE [3]. The solver is a cell-centered finite volume code with added artificial dissipation. State of the art acceleration techniques for the resolution of steady flows, such as implicit residual smoothing, W-cycle multigrid and local time stepping, are implemented. The proposed approach relies on the addition of a proportional feedback control and a low-pass filter to the system of equations to damp targeted frequencies. This method, developed for the computation of a steady solution of an unstable system [1,2], is here applied to steady case computations, specifically to enhance the convergence rate of the latter. Significant improvements in the convergence rates were found with and without the use of conventional acceleration techniques. This method is also applied on overset grid cases. A convergence speedup is observed in comparison to the reference case without SFD. This acceleration is important since the multigrid technique loses its efficiency on overset grids. The paper will present the implementation of the SFD algorithm in the NSCODE solver. A demonstration of the method on documented application cases from the literature will be performed. Then, the acceleration results on Euler cases with and without multigrid will be presented. Emphasis will be put on overset grids for which the methods show great promise for significant computational time reduction. Reference: [1] Jordi, B. E., Cotter, C. J., & Sherwin, S. J. (2014). Encapsulated formulation of the selective frequency damping method. Physics of Fluids, 26(3), 034101. [2] Richez, F., Leguille, M., & Marquet, O. (2016). Selective frequency damping method for steady RANS solutions of turbulent separated flows around an airfoil at stall. Computers & Fluids, 132, 51-61. [3] Pigeon, A., Taillon-Levesque, A., & Laurendeau, E. (2014). Two-Dimensional Navier-Stokes flow solver developments at École Polytechnique de Montréal. In CFD Society of Canada 22nd Annual Conference.

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Title: Toward a Hierarchically Task-Parallel, Multiscale Generalized Finite Element Method

Author(s): *Julia Plews, *Sandia National Laboratories*.

This presentation will demonstrate recent developments on a hierarchical multiscale generalized finite element method with global–local enrichment functions (GFEMgl). GFEMgl simultaneously resolves fine-scale (e.g., crack- or material-scale) and coarse-scale (e.g., component- or structural-scale) physics in interdependent local and global boundary value problems. Local solutions are inserted into the global basis as enrichment functions to achieve strong coupling of fine- and coarse-scale response without sacrificing fine-scale fidelity. Local problems may be subdivided and solved in parallel, which has shown promising scalability on shared memory computers while maintaining good accuracy relative to direct simulation [1,2]. However, scalable strategies targeted at the next generation of manycore high-performance computing platforms must exploit a combination of distributed parallel communication and on-node thread parallelism. Additionally, many engineering problems exhibit important phenomena which span more than two disparate length scales, for example, encompassing structural-, component-, and local material-scale response. The talk will focus on recent progress toward introducing a hierarchy of fine scale problems in the GFEMgl in order to consider multiple length scales of interest and exploit heterogeneous, task-based parallelism. [1] D.-J. Kim, C. Duarte, and N. Sobh. Parallel simulations of three-dimensional cracks using the generalized finite element method. Computational Mechanics, 47(3):265–282, 2011. [2] J. Plews and C. Duarte. Bridging multiple structural scales with a generalized finite element method. International Journal for Numerical Methods in Engineering, 102(3–4):180–201, 2015.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Micromorphic Computational Homogenization Framework for Heterogeneous Materials

Author(s): Raja Biswas, *Leong Hien Poh, *National University Singapore*.

The conventional first-order computational homogenization approach is restricted to problems where the macro characteristic length scale is much larger than the underlying Representative Volume Element (RVE). In the absence of a clear separation of length scales, higher-order enrichment is required to capture the influence of the underlying rapid fluctuations, otherwise neglected in the first-order framework. In this contribution, focusing on matrix-inclusion composites, a novel computational homogenization framework is proposed such that standard continuum models at the micro-scale translate onto the macro-scale to recover a micromorphic continuum. Departing from the conventional FE2 framework where a macroscopic strain tensor characterizes the average deformation within the RVE, our formulation introduces an additional macro kinematic field to characterize the average strain in the inclusions. The two macro kinematic fields, each characterizing a particular aspect of deformation within the RVE, thus provide critical information on the underlying rapid fluctuations. The net effect of these fluctuations, as well as the interactions between RVEs, are next incorporated naturally into the macroscopic virtual power statement through the Hill-Mandel condition. The resulting formulation recovers a micromorphic continuum at the macro-scale, instead of being postulated a priori. The length scale parameter associated with the higher-order term characterizes the nonlocal interaction between neighbouring micro-mechanisms within a RVE, which in turn provides a regularization effect and enables an accurate prediction of the size-effect. The micromorphic framework requires only C0 continuity for the basic field variables, enabling a straightforward numerical implementation. The excellent predictive capability of the proposed homogenization approach is illustrated through two examples, benchmarked against reference solutions obtained from direct numerical simulations. Considering a shear wave loading problem, it is shown that the homogenized micromorphic model adequately captures the material responses, even in the absence of a clear separation between the loading wavelength and the RVE size. A shear localization problem illustrates a regularizing effect of the micromorphic approach. In the presence of large spatial gradients spanning across only a few RVEs, an accurate shear band is predicted, in contrast to an erroneous localized deformation obtained with the first-order computational homogenization approach. For the examples considered, it is furthermore demonstrated that the homogenized solutions are independent on the choice of the underlying RVE for a given microstructure.

14th U.S. National Congress on Computational Mechanics
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Title: Automated Method for Mechanical Properties Characterization in Tissue-Engineered Cartilage

Author(s): *Ophelie Pollet, Aurelie Levillain, Thierry Hoc, *LTDS UMR 5513*; Christel Henrionnet, Astrid Pinzano, *IMoPA UMR 7365 CNRS*; Morad Bensidhoum, *B2OA UMR 7052*; Caroline Boulocher, *VetAgro-Sup*.

The importance of age as a factor when designing cell-based therapies for older patients is crucial since aging has been found to affect stem cells proliferation and differentiation potential. However the effect of aging on tissue-engineered cartilage properties especially mechanical properties has been underinvestigated. The objective of the study was to evaluate tissue-engineered cartilage architectural and mechanical properties according to patient age. A viscoelastic model was developed to calculate the mechanical properties in an automatic way, without impact of the manipulator. To determine the effects of patient age on cartilage synthesis, collagen sponges were seeded with mesenchymal stem cells from young patients (<20 yo) or old patients (>60 yo) during 28 days in chondrogenic medium. Histology was used to determinate the quality and quantity of cartilage extracellular matrix (ECM): collagen type II and GlycoAminoGlycanes (GAGs). Nanoindentation technique was used to study mechanical properties obtained by the force-displacement relationship. Cartilaginous graft from tissue-engineering was characterized using an indentation-relaxation test carried out with a spherical sapphire tip. Being a viscoelastic material, the graft was represented by a succession of springs and shock absorbers. Both instantaneous and equilibrium moduli were calculated from the relaxation modulus obtained using the hertzian contact (optimized with an integral operator) for a linearly viscoelastic material. As a term in this equation cannot be integrated analytically, the relaxation function was determined with a numerical solution using the Matlab algorithm fmincon. The algorithm was created to take into account the variation of the contact area under the tip during the experiment as well as the relaxation during the charge phase of the sample. For the first time, the effects of patient age on tissue engineering cartilage mechanical properties were studied. No differences in mechanical properties were found between young and old groups. Histology showed a greater synthesis of cartilaginous ECM by cells of old patients than by cells of young patients. We hypothesize that the cells derived from young patients were more “active” with a preference for multiplication rather than for differentiation as opposed to cells derived from old patients. We are currently investigating the effect of patient age in an animal model. In the near future, the algorithm will be used to characterize in an automated manner the mechanical properties of viscoelastic materials.

14th U.S. National Congress on Computational Mechanics
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Title: Coarse-Grained Accelerated Molecular Dynamics

Author(s): *Mauricio Ponga, *University of British Columbia*.

Molecular Dynamic (MD) simulation has proven to be a useful tool to understand many phenomena at the nanoscale. Although the capabilities of MD simulations for predicting properties of systems with great accuracy, many limitations still hinder widespread usage of this technique. One such limitation is the time scale that can be accessed with this technique. Since MD needs to resolve the thermal phonon vibrations of atoms and molecules, the critical time for conditional stability -the maximum time step that can be taken in order to maintain stability in the system- in the simulations is a fraction of this frequency. This, in turn, gives a critical time step of the order of 1 fs. The restriction in the time scale places several limitations in the total time that can be modeled with MD and, therefore, the loads and deformation are usually applied at exceedingly large rates that do not represent most of the everyday working condition of systems and components. In this work, a new technique for time acceleration of Molecular Dynamic (MD) simulations is proposed. The new technique is based on the concept of macroscopic evolution of systems at finite temperature and acceleration of rare events by phase space sampling at accelerated rates. We show how the free energy of the system for a given temperature can be computed by making a separation of slow-fast variables of motion and subsequent phase average. The proposed free-energy in terms of macroscopic -or expected values- of the atomic positions and momenta shows a much softer landscape than the original free-energy in terms of the instantaneous values, promoting a much faster transition rate than the regular MD simulation. The evolution of the free-energy at the desired temperature computed in terms of the macroscopic variables of the system can then be sampled at a much higher rate by using an artificial larger temperature, therefore greatly accelerating the time scale of the MD simulations and the transition rate of rare events. Several validation cases are studied to show the acceleration of MD simulations in relevant problem of interest such as, dislocation climb, vacancy diffusion, and vacancy cluster collapse in dislocation cores.

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14th U.S. National Congress on Computational Mechanics
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Title: Modeling of Electromechanical Composite Interfaces in the Material Point Method Using Cohesive Zones

Author(s): Adarsh Chaurasia, *University of Georgia*; Gary Seidel, *Stefan Povolny, *Virginia Tech*.

The current work is focused on extending the semi-meshless Material Point Method (MPM) to allow for interfacial discontinuities for solving boundary value problems (BVP) with composite interfaces. MPM follows an Eulerian - Lagrangian formulation allowing for transport of material points which carry the physical attributes of the material over a background computational mesh composed of finite elements. This allows for large deformation of the material without issues like mesh entanglement or singular matrices which would be expected in conventional finite element methods for such problems. In its traditional form, the MPM solution scheme does not allow for discontinuities in the solution of the field variables (e.g. composite problems) because the basis functions for the background mesh are continuous and differentiable over the entire domain. In the current work, we propose a solution scheme where multiple sets of basis functions are utilized and are associated with each phase of the composite. The sets of equations obtained for each phase are coupled to each other through a mathematical formulation which relies on cohesive zone modeling techniques as applied in finite element solutions. It is observed that the proposed framework allows for material discontinuity and reduces the fluctuations in field variables across the composite interface significantly. The results obtained from the proposed cohesive zone material point method (CZMPM) are compared against cohesive zone finite element modeling in terms of averaged field variables for two different test problems. The averaged field variables are chosen since they determine the homogenized effective properties of the composite materials. It is observed that the proposed CZMPM outperforms the traditional MPM significantly in terms of averaged errors in field variables specially for small number of background mesh elements. As a demonstration of an application, the proposed CZMPM is extended to model Carbon Nanotube (CNT)-polymer nanocomposite piezoresistive (i.e. change in effective resistivity with applied deformation) response with an electromechanical description of the CNT-polymer interface. The electromechanical nanocomposite modeling requires extension of the CZMPM model discussed to electrostatic BVP and interfacial description. The effective piezoresistive properties of nanocomposite are evaluated using micromechanics based homogenization of the representative volume elements. It is observed that the proposed electromechanical CZMPM model provides results close to an equivalent finite element model for small strains, but allows for solving large deformation problems because of particle based description of the material.

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Title: A Domain Decomposition Based Hybrid Framework for High Dimensional Stochastic Mechanics Problems

Author(s): *Srikara Pranesh, Debraj Ghosh, *Indian Institute of Science*.

In probabilistic mechanics the heterogeneity in material properties is often modeled using random fields. For computational purpose these random processes or fields need to be discretized. The Karhunen-Loeve (KL) decomposition is one of the widely used discretization method, where the eigenfunctions of the covariance kernel are used as the bases. Finding these eigenfunctions requires solving a Fredholm integral equation of second kind. The number of bases used in the approximation of random fields depends on the decay of the eigenvalues of KL expansion. For a covariance kernel, which has a dependence on the correlation length, it is known that a lower correlation length leads to slower decay of eigenvalues and vice-versa. Further, to propagate the uncertainty in the system, stochastic Galerkin (SG) is a very computationally efficient method. However, even for moderately high stochastic dimensionality, it suffers from the `curse of dimensionality'. Monte carlo simulation (MC) is dimension independent but is extremely expensive. These issues are addressed in this work in following steps, (i) For a general convariance kernel, we show that eigenvalues decay faster with reduction in domain size. (ii) Then, based on these results and previous results we propose a hybrid - combining MC and SG - domain decomposition based algorithm, to solve probabilistic mechanics problems with high stochastic dimensionality. In the first part of the work we derive bounds on the eigenvalues of KL expansion and numerical demonstrate there validity. Later using the proposed hybrid framework we solve a large three-dimensional elasticity problem with moderately high stochastic dimensionality of twenty five.

14th U.S. National Congress on Computational Mechanics
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Title: An Embedded Mesh Coupling of Overlapping Lagrange and ALE Meshes with Unilateral Type Contact Constraints

Author(s): *Mike Puso, Paul Tsuji, Ben Liu, Ed Kokko, *Lawrence Livermore Nat'l Lab*.

Coupling overlapping meshes typically in the form of a Lagrangian foreground and Eulerian or ALE background mesh has been shown to be very useful for simplifying model development and solving difficult fluid structure interaction problems. To this end, there are many different coupling techniques: immersed boundary, fictitious domain, embedded mesh etc. Each of these methods differ by how the constraint is computed and enforced (e.g. penalty, Lagrange multipliers, Nitsche etc.) Here, the embedded mesh approach from [1,2] using a stabilized Lagrange multiplier method is extended to allow contact type constraints. This would allow for potential gap openings and friction. This approach would be useful for applications such as extrusion type metal forming, earth penetration etc. Such examples will be demonstrated along with some aspects of the parallel implementation and performance. [1] M. Puso, J. Sanders, R. Settgast, and B. Liu “An Embedded Mesh Method in a Multiple Material ALE”, Computer Methods in Applied Mechanics and Engineering (15) 245-246, pp.273-289, (2012). [2] M. Puso, E. Kokko, R. Settgast, J. Sanders, B. Liu “An Embedded Mesh Method: Mathematical and Numerical Aspects” International Journal for Numerical Methods in Engineering 104 697-720, (2015).

14th U.S. National Congress on Computational Mechanics
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Title: Space-Time Boundary Element Methods for Dynamic Trusses

Author(s): *Dominik Pölz, Michael Helmut Gfrerer, Martin Schanz, *Graz University of Technology*.

The design of truss systems plays an important role in many engineering applications. Nowadays, the behaviour of such systems in the static case is well-understood. However, the recent past has seen a renewed interest in the dynamic case, which is even for trusses still subject of research. Most approaches to simulating dynamic truss systems employ a domain-based method for the spatial discretization in conjunction with a time-stepping scheme. In contrast, time-domain boundary integral equations of these problems eliminate the spatial discretization since they represent the solution by a fixed number of functions in time only. Space-time discretizations of these equations yield methods that impose little requirements on the smoothness of the solution and allow local refinement. Thus, the features of the solution, e.g. wavefronts, can be resolved properly. This talk is basically organized in two parts. First, the boundary integral equations of the elastic rod are discussed. This formulation is expanded to truss systems by means of continuity and equilibrium conditions at the nodes of the truss. The second part of the presentation is dedicated towards space-time discretizations of these boundary integral equations. A simple, yet powerful, a posteriori error estimator is employed to come up with an adaptive refinement. Numerical experiments verify the implementation by confirming the convergence of the method. Finally, a truss is simulated, illustrating the locality of the adaptive refinement.

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Title: The Properties of Dislocation Cores in Refractory Body-Centered Cubic Metals Affected by Ideal Strength Behaviors

Author(s): Chaoming Yang, Yongjie Hu, *Liang Qi, *University of Michigan*.

Group 5 and 6 refractory metals (such as Nb and Mo) are candidates as structural materials in many high-temperature application fields. Although most of them have the body-centered cubic (bcc) lattice and similar electronic structures, their individual dislocation core structures and properties are quite different, which results in different macroscopic plastic behaviors. The variations of dislocation core properties could result from the ideal strength behaviors of the corresponding perfect bcc crystals under extreme deformation conditions, which are strongly affected by the electronic structures such as the Fermi level. Here we apply first-principles calculations and atomistic simulations to investigate the dislocation core structures of these metals in order to build the quantitative connections between the ideal strength behaviors and the properties of dislocation cores. On the one hand, we perform detailed analyses of dislocation core structures and their motion mechanisms of those bcc metals by first-principles calculations to explore the origins of their variations from their ideal strength behaviors. On the other hand, we generate empirical atomistic potentials of these bcc refractory metals, which can accurately describe the ideal tensile and shear strength properties. The empirical potentials are applied to investigate the dislocation cores and the results will be compared with their counterparts from direct first-principles calculations. These results, combined with electronic structure analyses on the ideal strength behaviors, can be used to identify the most critical properties to determine the dislocation structures and macroscopic mechanical properties for future alloy design.

14th U.S. National Congress on Computational Mechanics
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Title: A Computational Study on Multi-Physics Coupling Effects in Ultrashort-Pulse Laser Material Processing

Author(s): *Dong Qian, Mohammad Rezaul Karim, Zhenpeng Qian, *University of Texas at Dallas*.

With the recent advances in laser-based manufacturing, there is a continuing interest in exploring the fundamental mechanisms of laser-material interaction to improve the performance of diverse engineering applications. The unique spatial and temporal profiles of lasers provide a wide range of capabilities for material processing and device fabrication. As an example, ultrashort pulsed lasers have been employed to meet the demands of applications such as drilling, ablation, volume structuring, etc. With the unique thermomechanical loads induced by the femtosecond laser, the effect on the microstructural evolution remains an active area of study, particularly when such effects are coupled with various micro and nanostructures. In this context, a multiscale simulation method that integrates the atomistic with continuum representations was established with a goal to link the relevant length scales. Efforts in applying the multiscale computational framework for laser material interaction will be presented in this talk. The technical implementation involves two key aspects: the first is in terms of integration of the electrons and phonons representation through the two-temperature model (TTM). The second is the multiscale representation of the atomistic and continuum degree of freedoms. Based on the multiscale framework, possible mechanisms of microstructural evolution, such as dislocation nucleation and propagation, and generation of defects, merging of particles are studied in detail.

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Title: Understanding the Effect of Head Shape on Traumatic Brain Injury Prediction due to Blast Loading

Author(s): Kirubel Teferra, X. Gary Tan, Athanasios Illiopoulos, John Michopoulos, *US Naval Research Laboratory*; *Siddiq Qidwai, *National Science Foundation*.

Detailed finite element (FE) modeling of the human head subjected to blast loading scenarios currently provides the only viable means to quantify mechanical response within the brain for traumatic brain injury (TBI) prediction. Although the exact relation between tissue mechanical response and injury is still quite unknown, the exceedance of threshold values based on direct and derived measures of stress, strain and acceleration within the brain are commonly used as injury criteria. Preliminary parametric studies varying head morphology and material properties of head components have shown significant variation in the predicted injury response, yet an established relationship of the effect of geometry and material properties on mechanics-based injury response metrics has yet to be determined. In this study, hundreds of finite element models comprised of accurate head morphologies are batch-generated, and their responses to blast loading are simulated in order to extract the range of injury prediction metrics due to morphology variation. Data of head morphology is obtained from the International Consortium for Brain Mapping (ICBM) database, which is a collection of serial section grayscale images (e.g. magnetic resonance images (MRIs)) of human heads. The data is evenly distributed between gender while the ages of the subjects range from 20-70. These 3D images are segmented using BrainSuite(R) to extract masks for the brain and the whole head. The DARTEL algorithm [1] is used to warp a template head to each one of the subjects. The template used is a high-resolution whole head T1-weighted MRI dataset of a healthy 26 year old male, representing the 50th percentile Caucasian male, which has been manually segmented using Simpleware ScanIP (Synopsys, Mountain View, USA) to identify 33 unique tissue regions [2]. For the purposes of this study, the regions have been aggregated into four components: skin, skull, CSF, and brain. All materials are modeled as linear viscoelastic except the brain, which is modeled as hyper-viscoelastic. The surface meshes of the various components of the templated model are warped, and tetrahedral FE meshes are auto-generated using Gmsh. FE analysis is done using multi-physics software CoBi, which models blast loading through CONWEP model. Various injury metrics are subsequently evaluated, along with an investigation into the key morphological features causing their variation. References: [1] J. Ashburner. Neuroimag. 38-1 (2007) p. 95. [2] R.T. Cotton, C.W. Pearce, P.G. Young, N. Kota, A.C. Leung, A. Bagchi, and S. Qidwai, Comput. Methods Biomech. Biomed. Engin. 19 (2015) p. 1.

14th U.S. National Congress on Computational Mechanics
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Title: Multiscale Computational Design of Bio-Inspired Materials with Advanced Mechanical Functions

Author(s): *Zhao Qin, *MIT*.

Mother nature presents many biological materials of sophisticated architectures and advanced mechanical properties, including spider webs, nacre, bamboo and so forth. In this talk, we will introduce our recent progress in using multiscale computational modelling tools to explore the structure-function relationships of these biological materials from the most fundamental scale level and up, and thereafter design and make bio-inspired composite materials that reach strength, toughness and lightweight features beyond conventional bulk materials. We will focus on the progress of our recent silk study and use it as an example to demonstrate how computational modelling can be used to guide the geometry and conditions for 3D printing and other advanced experimental synthesis methods to facilitate our capability of material design. Inspired by natural silk materials, we have been recently working toward designing structural porous materials of sufficient strength and uniform porosity with lightweight properties, making them suitable for higher mechanical forces with less material use. Our work has demonstrated that by using coarse-grained models built based on knowledge learned from atomistic models, we can predict material functions and optimize the design accordingly. Our results have shown that silk reinforced composites are leading to designs of efficient porous membrane materials with useful mechanical resilience for solvent filtration. Altogether, our study provides efficient tools to design bio-inspired materials with complex network architectures for desired mechanical functions and low density to meet critical biomechanics applications.

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Title: Analysis of a Mixed Discontinuous Galerkin Method for Incompressible Magnetohydrodynamics

Author(s): *Weifeng Qiu, *City University of Hong Kong*.

In this paper we propose and analyze a mixed DG method for the stationary Magnetohydrodynamics (MHD) equations with two types of boundary (or constraint) conditions. The numerical scheme is based a recent work proposed by Houston et. al. for the linearized MHD. With two novel discrete Sobolev embedding type estimates for the discontinuous polynomials, we provide a priori error estimates for the method on the nonlinear MHD equations. In the smooth case, we have optimal convergence rate for the velocity, magnetic field and pressure in the energy norm, the Lagrange multiplier only has suboptimal convergence order. With the minimal regularity assumption on the exact solution, the approximation is optimal for all unknowns. To the best of our knowledge, this is the first a priori error estimates of DG methods for nonlinear MHD equations.

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Title: Magnetophoretic Interaction of a Pair of Ferrofluid Droplets in a Rotating Magnetic Field

Author(s): *Mingfeng Qiu, James Feng, *University of British Columbia*; Shahriar Afkhami, *New Jersey Institute of Technology*; Ching-Yao Chen, *National Chiao Tung University*.

A ferrofluid is a stable suspension of magnetic nano-particles in a suitable carrier fluid. The ultra-fine particles and the colloidal stability make the ferrofluids behave as a homogeneous medium, while displaying a variety of novel phenomena under an external magnetic field. In the past decades, thorough knowledge on a single droplet under the influence of a rotating field has been obtained. However, the interaction of multiple droplets has received much less attention. Recent experiments have discovered a mode of planetary motion of a pair of ferrofluid droplets in a rotating magnetic field. It consists of the self-spin of individual droplets and the revolution of the pair around each other with a phase lag from the rotating field. In this study, we explore this phenomenon using direct numerical simulations. An open source software Gerris (http://sf.gfs.net) is employed. The package features adaptive mesh refinement on a structured quad-/oct-tree grid, a volume-of-fluid formulation of the interface between the ferrofluid and the surrounding liquid, and an accurate computation of the surface tension. Direct simulations have reproduced the key features of the experiments. We observe that the center of mass of droplets oscillates in both radial and angular directions during the planetary motion. We show that the frequency of the oscillations is dictated by the periodical change of phase lag between the pair and the rotating field, which agrees well with the experimental observations. It is also discovered that with increasing frequency of the driving field, the angular velocity of the pair increases as a result of enhanced hydrodynamic interaction between the deformed droplets. Besides planetary motion, a droplet-locking regime is discovered under certain operating parameters. In the locking regime, individual droplets stick together and rotate in phase with the driving field, while maintaining a thin film between them.

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Title: Tetmesh Scaling for Solution Verification

Author(s): *William Quadros, Brian Carnes, *Sandia National Labs*.

This abstract proposes an approach for generating a series of meshes from an input tetmesh for performing solution verification for finite element analysis. Solution verification normally requires refinement studies to verify convergence. To facilitate this, multiple meshes with different resolutions are generated using the standard templates of uniform mesh refinement (UMR). For tet elements, this can result in 8X and 64X the number of initial elements in just one and two levels of refinement, respectively, and can quickly become too computational expensive for most practical use. We also note that UMR cannot be used for coarsening the mesh to create meshes with fewer numbers of elements. For our application, the input mesh generally contains multiple volumes with different local element sizes and gradation that is achieved by specifying nodal spacing followed by post-meshing operations such as local refinement and smoothing. In this work, we propose a tetmesh scaling procedure that allows the user to generate a series of meshes for solution verification from an initial mesh. Element counts produced are roughly controlled based on selected user-defined scale factors. The resulting scaled meshes preserve characteristics such as relative local element sizes and gradation throughout the domain. The tetmesh scaling procedure first extracts the skin of the input tetmesh to define a mesh-based B-rep geometry. If the input tetmesh has multiple material groups of elements, an assembly model with multiple geometric volumes is constructed. Next, a mesh size field is built by capturing the input mesh characteristics. The mesh characteristics such as local size and gradation can be measured using the element edge lengths throughout the domain. The average edge length at every node is calculated and stored on either a background tetmesh (i.e., a copy of input tetmesh) or on a background octree grid. This size field can then be scaled using a user specified arbitrary positive scale factor to globally increase or decrease the mesh size. A user-defined scale factor greater than 1.0 will refine the mesh while a scale factor between 0.0 and 1.0 will result in coarsening. This procedure also supports different user-defined scale-factors on different volumes, which is followed by gradient limiting to obtain smooth transition between the volumes. Finally, the surfaces and interior of the assembly model is meshed using the common mesh size field. Thus, a series of meshes with user-controlled element budgets can be generated for facilitating efficient solution verification.

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Title: A Galerkin Isogeometric Method for Karhunen-Lo■eve Approximation of Random Fields

Author(s): *Sharif Rahman, *The University of Iowa*.

Much of the progress in uncertainty quantification of complex mechanical systems has been made at the expense of speaking two disjointed mathematical languages: the vocabulary of computer-aided design (CAD) for geometric modeling and the lexicon of finite-element analysis (FEA) for computational mechanics, including stochastic analysis. As a consequence, the geometry-to-mesh mapping is neither automatic nor differentiable, creating a major bottleneck in the uncertainty quantification process, especially for industrial-scale problems. The isogeometric paradigm crosses the divide by changing from classical FEA to a solely CAD-based analysis procedure, tightly integrating geometry, meshing, and analysis in the same footing [1]. While the power of isogeometric analysis has been demonstrated in the literature, deterministic conditions are often employed, meaning that the uncertainties of loads, geometry, and material properties are disregarded. Therefore, a stochastic version of the isogeometric framework is essential to Verification and Validation - an important goal of computational mechanics. This paper presents a Galerkin isogeometric method for solving a Fredholm integral eigenvalue problem, leading to random field discretization by the Karhunen-Loeve expansion. The method involves a Galerkin projection onto finite-dimensional a subspace of a Hilbert space, basis splines (B-splines) and non-uniform rational B-splines (NURBS) spanning the subspace, and standard methods of eigensolutions. Compared with the existing Galerkin methods, such as the finite-element and mesh-free methods, the NURBS-based isogeometric method preserves exact geometrical representation of the physical or computational domain and exploits regularity of basis functions delivering globally smooth eigensolutions. Therefore, the introduction of the isogeometric method for random field discretization is not only new, but it also offers a few computational advantages over existing methods. In the big picture, the use of NURBS for random field discretization enriches the isogeometric paradigm. As a result, an uncertainty quantification pipeline of the future can be envisioned where geometric modeling, stress analysis, and stochastic simulation are all integrated using the same building blocks of NURBS. Three numerical examples, including a three-dimensional random field discretization problem, illustrate the accuracy and convergence properties of the isogeometric method for obtaining eigensolutions. [1] J. A. Cottrell, T. J. R. Hughes, and Y. Bazilevs. Isogeometric Analysis: Toward Integration of CAD and FEA. John Wiley & Sons, 2009.

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Title: An Adaptive Cohesive Zone Model for Fatigue Crack Growth in the Framework of Generalized Plasticity

Author(s): *Noémie Rakotomalala, *Safran Tech*; Vincent Chiaruttini, *Onera*.

The safety restrictions in aeronautical industry have led to an increased interest in Damage Tolerance analysis. This consists in considering the presence of a structural defect and verifying that the growth of this defect will not have disastrous in-flight consequences. Accurate lifetime prediction of critical engine parts, such as combustion chambers, requires the use of 3D crack growth analysis accounting for various physical interactions. Indeed, cracks initiated near holes undergo strong thermal and mechanical gradients combined with multiaxial fatigue loading and environmental effects, such as hot gas corrosion. This work is motivated by the development of a robust 3D crack growth simulation that can be applied in the framework of generalized plasticity. It is well-known that the Paris law and similar models are valid under ideal conditions (linear elastic fracture mechanics, long cracks, constant amplitude loading, and small-scale yielding). Those models are widely used to perform 3D crack growth simulations under fatigue loading using numerical methods mostly based on X-FEM/Levelset methods or remeshing techniques. When these ideal conditions are not met, the predictive capability of these approaches is questionable. In this work, an alternative approach based on cohesive theories of fracture is explored, combined with an explicit resolution of the near-tip plastic fields and the enforcement of closure effect as a contact constraint. In order to represent the fatigue phenomena, an irreversible cohesive law is used to simulate cyclic dissipative mechanisms controlled by an appropriate internal variable. Also, the crack path is discretized using mixed finite interface elements, which are formulated based on an augmented Lagrangian [1]. The plastic dissipation related to the crack growth is computed explicitly in the bulk, and computed independently of the cohesive separation processes; it will not be lumped into the crack propagation criteria. However, allowing discontinuities between each bulk element does not converge and results in mesh dependency. We address this by using advanced remeshing techniques enhanced to allow the dynamic insertion of cohesive elements [2]. We will present the numerical approach and its validation by looking into the fracture pattern for different prescribed crack paths. References: [1] E. Lorentz, A mixed interface finite element for cohesive zone models, Computer Methods in Applied Mechanics and Engineering, 2008, 198, 302-317. [2] V. Chiaruttini, D. Geoffroy, V. Riolo, M. Bonnet, An adaptive algorithm for cohesive zone model and arbitrary crack propagation, European Journal of Computational Mechanics, Volume 21, Issue 3-6, Pages 208-218, June 2012.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Mesodynamics - A Hybrid Deterministic-Statistical Framework for Molecular Dynamics

Author(s): *Amuthan Ramabathiran, Michael Ortiz, *Caltech*; Pilar Ariza, *Universidad de Sevilla*.

We present a new computational framework, Mesodynamics, for temporal coarse-graining of non-equilibrium atomistic simulations. Current techniques for atomistic simulation involve either fully deterministic methodologies like Molecular Dynamics, or stochastic approaches based on Statistical Mechanics like Monte Carlo methods. Our work is motivated by the need for a robust computational framework that seamlessly transitions between deterministic, particle-based descriptions and statistical, probability distribution-based descriptions to capture the multi-scale physics of atomistic systems. Mesodynamics generalizes previous work in this direction like the finite temperature quasi-continuum method [1] and provides a sound mathematical basis for coarse-graining in time, thereby permitting the study of atomistic systems with multiple time scales. We accomplish this in two stages: first, we present a new variational principle for phase space probability distributions involving a weak formulation of the Liouville equation that provides a rigorous mathematical basis for describing the time evolution of atomistic systems, and second, we restrict the phase space distributions in the variational principle to a class of maximum entropy distributions to render the framework computationally tractable. Mesodynamics further provides a tool for studying the non-equilibrium behavior of atomistic systems since it naturally contains a means to treat internal heat transfer due to spatial thermal inhomogeneities. We present applications of the new framework to a variety of problems spanning multiple time scales, like the approach to equilibrium in atomic clusters and the time evolution of atomic clusters composed of elements with disparate masses. The implementation of Mesodynamics presents fresh challenges related to the calculation of high-dimensional phase integrals. We discuss various numerical strategies that we employed to overcome this computational bottleneck. We also outline the formal connection of Mesodynamics to a rigorous description of the statistical behavior of Hamiltonian systems using the Theory of Optimal Transport. In particular, we elucidate the Wasserstein geometry of the space of probability measures as the natural mathematical setting for Mesodynamics, and discuss the generalizations and implications of this approach for developing time coarse-graining strategies for non-equilibrium atomistic simulation. [1] Venturini G, Wang K, Romero I, Ariza MP and Ortiz M, Atomistic long-term simulation of heat and mass transport, J. Mech. Phys. Solids (2014), 73, 242–268.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Hierarchic Isogeometric Large Rotation Shell Elements Including Linearized Transverse Shear Parametrization

Author(s): *Ekkehard Ramm, *Inst. for Str. Mech., UofSt*; Bastian Oesterle, Renate Sachse, Manfred Bischoff, *Institute for Structural Mechanics, University of Stuttgart*.

Isogeometric Analyses using NURBS functions enable a smooth surface description with higher inter-element continuity which opens up new possibilities in the analysis of thin-walled structures. An important advantage is the straightforward implementation of classical theories, which require C1-continuity, e. g. Kirchhoff-Love shell formulations, as demonstrated in [1]. Based on these simplest models, also shear deformable theories, like Reissner-Mindlin shell formulations, can be formulated in an elegant way. In [2] a hierarchic set of isogeometric shell finite elements is developed for the geometrically linear case, a priori avoiding shear locking within the framework of a pure displacement formulation. In this contribution, two novel hierarchic isogeometric formulations for geometrically nonlinear shell analysis including transverse shear effects are presented (see also [3]). Both methods combine a fully nonlinear Kirchhoff-Love shell model with hierarchically added linearized transverse shear components. Thus, large rotations can be taken into account in a simple and straightforward way. The underlying assertion is that in practical applications the transverse shear angles are small, even for thick shells and large deformations. Various numerical experiments confirm this statement. The two presented formulations differ in the way the transverse shear effects are included. The first formulation makes use of hierarchic rotations, while the second formulation uses hierarchic shear displacements. The corresponding hierarchic setting results in an additive strain decomposition into parts resulting from membrane and bending deformation and additional contributions from transverse shear. It requires at least C1-continuous shape functions, which can be easily established within the isogeometric context based on NURBS, T-Splines, subdivision surfaces or other smooth spaces. This concept is intrinsically free from transverse shear locking. In the nonlinear case it dramatically facilitates representing large rotations in shell analysis. References [1] J. Kiendl, K.-U. Bletzinger, J. Linhard, R.Wüchner. Isogeometric shell analysis with Kirchhoff-Love elements. Computer Methods in Applied Mechanics and Engineering, 198:3902–3914, 2009. [2] R. Echter, B. Oesterle, M. Bischoff. A hierarchic family of isogeometric shell finite elements. Computer Methods in Applied Mechanics and Engineering, 254:170–180, 2013. [3] B. Oesterle, R. Sachse, E. Ramm, M. Bischoff. Hierarchic isogeometric large rotation shell elements including linearized transverse shear parametrization. Computer Methods in Applied Mechanics and Engineering, submitted.

14th U.S. National Congress on Computational Mechanics
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Title: Quantifying Microscale Damage through Image-Based Material Testing of Particulate Composites Using Micro-Tomography

Author(s): *Katherine Ramos, Andrew Gillman, Karel Matous, *University of Notre Dame*.

Understanding the mechanical behavior that arises from the heterogeneity at different length scales of natural and synthetic heterogeneous materials is essential. X-ray microcomputed tomography (micro-CT) has become a popular method in the materials science community for nondestructive analysis of the internal microstructure in these complex materials. In particular, this technology allows in situ analysis of materials under thermo-mechanical loading. The power of this experimental technique is enhanced through detailed statistical analysis of the evolution of various structural features through robust image processing strategies at various stages of loading. This work employs image-based modeling concepts alongside complex three-dimensional imaging techniques to understand the influence of microstructure and local damage phenomenon on the effective mechanical response of rubber-glass bead composites. In our work, a non-destructive, three-dimensional image-based analysis protocol which provides high fidelity of sample testing and data assessment has been established. An investigation was performed on various microstructure compositions of silicone rubber reinforced with silica particles. In situ compression experiments were used to study how the microscale damage (void creation from debonding/matrix tearing) develops and evolves in the context of four primary studies: i) effect of particle volume fraction ii) effect of particle diameter iii) local damage phenomena and it's evolution (incremental loading/unloading) and iv) effect of surface treatments on bonding characteristics. The rich data analysis collected from the various experimental studies offers an understanding of the complex phenomena attributing to the material's response to loading including the mechanical and morphological response of non-linear viscoelastic materials subjected to uniaxial compression. In addition to the fundamental understanding, these experiments serve as validation data sets for multi-scale modeling approaches. In particular, the analysis will serve as a foundation in the development of better constitutive theories for Finite Element Analysis (FEA) of these heterogeneous microstructures. The development of representative unit cells respecting the characteristic length scales, as determined through analysis of statistical correlation functions, will be established. Focus is placed on the development of non-linear viscoelastic constitutive models with damage/debonding for these complex heterogeneous systems. This analysis and framework yields new insight of these composite materials required for the optimal material design. Additionally, the thorough and reliable experimental and image processing pipeline established supplements existing image-based modeling techniques substantially.

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Title: A Continuous Mesh Model for Goal-Oriented hp-Adaptation

Author(s): *Ajay Rangarajan, Georg May, *RWTH Aachen University*.

In many applications high-order consistent numerical schemes using piecewise polynomial approximation have been recognized as advantageous. Nonlinear convection-dominated problems, such as compressible flow, are a notable exception. These problems usually exhibit highly anisotropic features, as well as low solution regularity, or even discontinuities. It is very desirable to reflect both the anisotropy, and varying regularity in the chosen numerical approximation space. In fact, anisotropic hp-adaptation is almost imperative in this context to realize the potential of high-order schemes, and a very carefully designed method is needed to adapt or even optimize the approximation space with respect to a given problem. This has impeded the development of high-order consistent numerical methods that are competitive with robust state-of-the-art tools. To improve the status quo, metric-based adaptation has emerged as a powerful paradigm. Metric-based methods encode simplex meshes in a pointwise varying tensor field, often termed a continuous mesh. Corresponding discrete meshes contain elements that are (nearly) equilateral under the Riemannian metric induced by the tensor field. We have previously proposed a method to obtain tailor-suited meshes based on analytic optimization of the metric field with respect to the numerical error measured in some integral norm. The significance of using a continuous mesh model is that analytic optimization is greatly simplified when operating on the metric field, rather than a discrete mesh. Our approach requires only a suitable error model, compatible with the continuous mesh. In the present work we deal with the extension of the concept to more general goal-oriented hp-adaptation in the context of convection-diffusion problems. Here, the objective of the optimization is the accurate computation of any solution-dependent functional, provided only that the functional is admissible with respect to an adjoint problem. Adding a suitably defined polynomial degree distribution function, we generate a continuous hp-mesh, and formulate an optimization problem in a weighted norm, where the weight comes from the adjoint solution, in order to minimize the error of the target functional. The proposed optimization method can be used with any numerical scheme using piecewise polynomial approximation, but is combined in the most straightforward way with schemes using discontinuous approximation spaces. In particular we present numerical results for various convection-diffusion problems using discontinuous Galerkin schemes.

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Title: A Flexible Conservative Remapping Framework for Exascale Computing

Author(s): Ondrej Certik, Ferenbaugh Charles, *Garimella Rao, Angela Herring, Chris Malone, *Los Alamos National Laboratory*; Chris Sewell, *Los Alamos National Laboratory (currently at Intuitve Surgical, Inc)*.

We present an open-source remapping framework called Portage that can transfer fields between general polyhedral meshes while conserving some integral quantity of interest. At the heart of Portage is a templated driver that can be constructed with any set of classelatet can perform the steps required in conservative remapping - searching, intersection and interpolation. The driver is also templated on classes for the mesh and state managers that can answer a specific set of queries. Distributed memory parallelism in Portage requires that the mesh and state managers support the concept of partitions surrounded by a halo of ghost elements. On-node parallelism in Portage requires the search, intersection and interpolation classes to be written such that that can operate on each element without any side effects. This allows Portage to use NVIDIA's Thrust interface to enable on-node parallelism using OpenMP, Intel TBB or CUDA backends. We have tested Portage in 2D/3D for remapping between general polygonal and polyhedral meshes. The code can remap cell-centered or node-centered variables using 1st or 2nd order accurate remapping with Barth-Jesperson limiting of gradients to enforce monotonicity. We will present convergence and scaling results. LA-UR-16-26956

14th U.S. National Congress on Computational Mechanics
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Title: Computational Models for Molten Corium Flow and Reaction with Concrete

Author(s): *Rekha Rao, Alec Kucala, Jeremy Templeton, David Noble, Yifeng Wang, Denise Bencoe, David Louie, *Sandia National Laboratories*.

The catastrophic nuclear reactor accident at Fukushima created a loss of confidence in nuclear energy and a demand for new engineered safety features that could mitigate or prevent radioactive material releases to the environment. We are working to understand the flow and solidification of molten corium after a core breach. The corium is made up of a mixture of ceramic (i.e., UO2, ZrO2 and FeO) and metal materials (i.e., Zr, Fe, Cr, and B) from structural supports, control rods, and fuel-cladding. . During a nuclear meltdown, the corium can reach temperatures above 2000oC. During a core breach, the corium escapes containment where it can react with the concrete floor of the reactor cavity. In this project, we seek to develop a model for the flow, solidification, and reaction of the molten corium as it reaches the floor of the cavity and begins to produce gases from interactions with concrete. The corium moves in a lava-like manner and voids appear where gas bubbles through the molten material. A modeling effort is underway to understand the time-scale of the flow and predict the final structure of the material. A new wetting model coupled to a conformal decomposition finite element method is used to predict the flow of the corium using a temperature-dependent viscosity to halt the flow. A simple extent of reaction is used to create gas from reactions of corium and concrete. Heat loss to the environment, including radiation, must be included to capture the phenomena of interest. Preliminary results from the model are shown and future modeling directions will be discussed. The information from the detailed physics-based model will be implemented as a reduced-order model for MELCOR, a widely used severe accident computer code. *Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: Model Reduction for Transport Problems via Nonlinear State Space Transformation

Author(s): Christoph Lehrenfeld, *University of Göttingen*; Mario Ohlberger, *Stephan Rave, *University of Münster*.

A well-known issue for reduced order modeling of transport phenomena with moving shock discontinuities, problems with moving internal interfaces or moving boundaries is the slow decay of the Kolmogorov n-widths of their corresponding solution manifolds (e.g. [1]). This means that there cannot exist linear low-order state approximation spaces in which the solution can be accurately represented for all times or parameters of interest. Thus, successful reduced order modeling of these problems necessarily has employ some form of nonlinear approximation of the solution. In this talk we present two such approaches, both based on transformations of the problem's underlying spatial domain. First, we show how standard reduced basis methods can be combined with the so-called 'method of freezing' approach [2] to derive efficient reduced order models for equivariant hyperbolic problems with moving shocks [3]. Second, we present recent work on reduced basis approximation of a parametric model for osmotic cell swelling, where we employ an ALE formulation to transform the moving cell volume to a fixed reference domain. [1] M. Ohlberger and S. Rave, Reduced Basis Methods: Success, Limitations and Future Challenges, in Proceedings of ALGORITMY, 2016, pp. 1-12. [2] W.-J. Beyn and V. Thümmler, Freezing solutions of equivariant evolution equations, SIAM J. Appl. Dyn. Syst., 3 (2004), pp. 85-116. [3] M. Ohlberger and S. Rave, Nonlinear reduced basis approximation of parameterized evolution equations via the method of freezing, C. R. Math. Acad. Sci. Paris, 351 (2013), pp. 901-906.

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Title: Geometric and Black Box Multigrid on Hybrid Architectures

Author(s): *Luc Berger-Vergiat Ray Tuminaro, *Sandia National Laboratories*.

In this work we propose to leverage the properties of structured grids often used in aerospace applications to improve the performance of linear solvers and preconditioners on hybrid computer architectures. Aerospace applications often involve the modeling of objects moving at high Mach numbers through a fluid. For hypersonic conditions, it can be challenging to develop a discrete representation of the fluid with unstructured meshes that will resolve problem features with an adequate level of accuracy. Instead, many simulation efforts rely on block structured or fully structured meshes to simulate such flight conditions. Structured and block structured meshes allow one to develop fast preconditioners such as geometric and black box multigrid algorithms that take advantage of the particular ordering of the unknowns to distribute the work load efficiently within and between compute nodes. Additionally, structured multigrid solvers generally give rise to much sparser coarse grid operators (and so less computational work) than their algebraic multigrid counterparts. Furthermore, the smoothers used to remove high frequency components of the error can also take advantage of the mesh structure. For instance, line solvers can be used to cheaply and effectively reduce the error in the normal direction to the moving body and careful ordering of an ILU algorithm can also yield improved efficiency at the smoother level. We will present implementation details of the above solver algorithms on hy- brid computer systems where classic inter-node parallelism is achieved using MPI and intra-node parallelism is implemented through Kokkos. Kokkos is a library aimed at providing a uniform interface to pthreads, OpenMp and CUDA, allowing us to test algorithms on a variety of heterogeneous architectures containing GPUs and co-processors. Finally comparisons of the two proposed multigrid algorithms will be provided along with comparisons to a standard algebraic multigrid solver. Special emphasis will be given to the ability of each algorithm to accurately capture the physics of the problem on coarse grids and to potential stabilization methods for the coarse grid operators. Overall convergence studies will be provided to assess the effectiveness of the approaches compared to off the shelf preconditioners and scaling properties will be demonstrated on large test cases.

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Title: A Stress Recovery Procedure for Cost-Effective Isogeometric Analysis of Composite Plates

Author(s): *Alessandro Reali, John-Eric Dufour, Alessia Patton, Giancarlo Sangalli, Ferdinando Auricchio, *University of Pavia*; Pablo Antolin, *École Polytechnique Fédérale de Lausanne EPFL*.

This work focuses on the development of an isogeometric method for composite plates taking advantage of the accuracy and high-regularity properties of isogeometric analysis to build a cost-effective stress recovery procedure. The proposed technique simulation strategy consists of using 3D isogeometric computations with a reduced number of elements in the thickness (namely, one) and a layer-wise integration rule, or, when possible, an homogenized approach, granting an inexpensive and accurate approximation of the in-plane response. This solution is then post-processed in order to obtain also an accurate stress state through the thickness, based on the integration of the equilibrium equations in strong form. Such an approach allows to drastically reduce the number of degrees of freedom and, accordingly, the overall computational time as compared to the standard full 3D layer-wise approach where every layer corresponds to an element through the thickness. The post-processing operation is in fact very fast and its cost does not increase significantly with the number of degrees of freedom. Several numerical experiments are shown, revealing the very good accuracy-to-cost ratio of the method, which appears to be particularly effective on composite stacks with a large number of layers. Finally, the isogeometric collocation version of the approach is also discussed.

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14th U.S. National Congress on Computational Mechanics
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Title: Image-Based Estimation of Mitral Valve Strains in the Beating Heart

Author(s): *Bruno Rego, Amir Khalighi, Andrew Drach, Michael Sacks, *University of Texas at Austin*; Joseph Gorman, Robert Gorman, *University of Pennsylvania*.

Each year, more than 40,000 people in the United States undergo surgery for mitral valve (MV) repair, frequently as a result of myocardial infarction (MI). Repair failure is a major problem, however, with 30% of patients experiencing recurrence of ischemic regurgitation within 6 months of surgery. In the present study, we examined how the mechanical properties and in-vivo geometry of the MV change after MI, in an effort to gain a deeper understanding of the driving factors behind post-MI valvular remodeling. In addition, we used our experimental measurements to inform an image-based method for estimating in-vivo strains across the MV leaflet. MI was induced in three adult Dorsett sheep, and 3D ultrasound scans were collected pre-MI, immediately post-MI, 4 weeks post-MI, and 8 weeks post-MI. At 8 weeks, animals were sacrificed and MV tissues were explanted for biaxial mechanical testing. In addition to examining the geometry of the valve directly, we have developed a framework to estimate in-vivo strains throughout the leaflet by integrating the ultrasound tracings into a finite element (FE) modeling approach. Briefly, the imaged open state of the valve is converted to an FE mesh, and closure is simulated using the measured mechanical properties of each specimen. Material properties and boundary conditions are then iteratively adjusted such that the simulation yields a close match to the imaged closed state, and final estimates for local strain are obtained. This methodology will be validated using an existing database of in-vitro fiducially labeled images of MV closure. Biaxial testing results showed that at 8 weeks post-MI, the mechanical properties of the MV anterior leaflet are severely disturbed. While normal MVs are much more extensible radially than circumferentially, this anisotropy is entirely reversed post-MI. Moreover, ultrasound scans showed that the MV annulus is substantially flattened post-MI and that the MV leaflets lose their normal tenting behavior during closure. Our results shed significant light on the extent to which disease can alter the mechanical and geometric properties of the MV, both of which greatly affect computational estimates of local strains. These findings are highly relevant to the design of MV repair devices and the optimization of surgical strategies. While current MV repair endeavors largely seek to return the valve to its pre-diseased state, our results suggest that this approach may not be favorable, and that an effort to place the MV in an alternative homeostatic state may lead to decreased repair failure.

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Title: Hex-Dominant Meshing

Author(s): Jeanne Pelerin, Amaury Johnen, Jonathan Lambrechts, *Jean-Francois Remacle, *UCL*.

This paper deals with a new approach for hex dominant meshing: 1) A 3D frame field is created through a PDE approach using the Ginzburg-Landau theory applied to spherical hamronics Y^j_4, j=-4,...,4. 2) Points are located in the domain in a frontal fashion using the directions of the frame field. 3) A tetrahedral mesh is created using the points. 4) A new algorithm is proposed for searching combinations of tetrahedra into hexahedra. The new algorithm allows to find more hexahedra than any other existing algorithm (patterns with 10 tetrahedra that form a valid hex are found). The same algorithm also finds prisms and pyramids. 5) An heuristic based on a deep learning approach is finally used to find a good solution to that maximal clique problem that allows to find a good set of compatible hexahedra. Examples of 3D hex-dominant meshes are presented together with finite element computations.

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Title: A Parallel Implementation of the Enhanced Local Pressure Model for the Large Scale Simulation of Hydraulic Fracturing

Author(s): *Ernst W. Remij, Joris J.C. Remmers, Jacques M. Hyughe, David M.J. Smeulders, *TU Eindhoven*; Erik Jan Lingen, *Dynaflow Research Group*.

Hydraulic fracturing, or fracking, is the process by which a crack propagates by applying a fluid pressure inside the crack. In geo-mechanics, this process is used to stimulate oil and gas reservoirs. Another application is the creation artificial wells with increased conductivity for Enhanced Geothermal Systems. The fracking procedure can be controlled by adjusting several parameters, such as the magnitude of the hydraulic loading and the viscosity and density of the pressurized fluid. In order to understand the effect of these parameters on the fracture process, in relation to the mechanical properties of the formation, numerical simulations can be of assistance. The starting point for developing a numerical model to predict crack growth in geo-mechanics is a poromechanical continuum model for a fully saturated medium in combination with a cohesive zone relation. In the recent years, the development of such models has concentrated on the application of the eXtended Finite Element Method, e.g. [1]. An extension of these models is the Enhanced Local Pressure model by Remij et al. [2], where the pressure in the fracture is described by an additional set of degrees of freedom. The pressure gradient due to leakage near the fracture surface is reconstructed analytically, based on Terzaghi's consolidation solution. As a result, relatively coarse meshes can be used and it is ensured that the injected fluid ends up completely in the existing pre-crack. The numerical model can be used to study the hydraulic fracturing process near natural faults and other cracks. However, due to the large differences in length-scales between the process zone and the dimensions of the rock formation, parallelization of the code is inevitable. In this paper, we will present the parallelization of the X-FEM based Enhanced Local Pressure model by using a domain decomposition strategy. Special attention is paid to the data management of the additional degrees of freedom and the calculation of the partition of unity enrichment functions. The resulting linear system of equations is solved in parallel using a GMRES algorithm in combination with a two-level preconditioner. The performance of the code is demonstrated by means of a number of realistic fracking simulations, including a case with multiple, interacting cracks. [1] R. De Borst et al. (2006) Archive of Applied Mechanics, 75(10), 595-606. [2] E.W. Remij et al. (2015) Computer Methods in Applied Mechanics and Engineering, 286, 293-312.

14th U.S. National Congress on Computational Mechanics
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Title: Stochastic Sensitivity Analysis for Reliability-Based Topology Optimization

Author(s): *Xuchun Ren, *1Department of Mechanical Engineering, Georgia Southern University, Statesboro, GA, 30458, USA*; Xiaodong Zhang, *State Key Laboratory of Bridge Engineering Structural Dynamics, China Merchant Chongqing Communications Research & Design Institute Co., Ltd, Chongqing,400067,China*.

The objective of this work is to develop efficient methods for stochastic sensitivity analysis for reliability-based topology optimization (RBTO). A new computational method is proposed for calculating topological sensitivities of failure probability of high-dimensional complex systems subject to random inputs. The proposed method, capable of evaluating stochastic sensitivities for large-scale RBTO problems, integrates a polynomial dimensional decomposition (PDD) of multivariate stochastic response functions and embedded Monte Carlo simulation. In addition, the failure probability and its topological sensitivities are both determined concurrently from a single stochastic analysis. When applied in collaboration with the gradient based optimization algorithm, the proposed methods afford the ability to solve industrial-scale RBTO design problems. Numerical examples indicate that the new methods provide not only theoretically convergent or accurate design sensitivities but also computationally efficient solutions.

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Title: Small- and Large-Deformation-Based Peierls-Nabarro and Phase-Field Modeling of the Dislocation Core in fcc Systems and Comparison with Atomistics

Author(s): *Jaber Rezaei Mianroodi, Bob Svendsen, *RWTH Aachen University*.

The purpose of this work is the development of continuum models for dislocation-mediated processes in nanocrystals. In particular, this is based on a detailed comparison of such models with each other as well as with atomistic modeling via molecular statics (MS) and molecular dynamics (MD). On the continuum side, the models of interest include generalized Peierls-Nabarro (GPN: Xiang et al., Acta Mat. 56, 1447-1460, 2008), phase-field dislocation dynamics (PFDD: e.g., Hunter et al., Phys. Rev. B 84, 144108, 2011), atomistic phase-field microelasticity (APFM: Mianroodi, Svendsen, JMPS 77, 109-122, 2015). As shown by Mianroodi et al. (JMPS 95, 719-741, 2016), GPN and PFDD are in fact (physically) equivalent. In contrast to MS and MD, all of these are geometrically linear models. Recently, PFDD and APFM have been extended to geometric non-linearity (Mianroodi, Svendsen, in preparation, 2017). Computational comparisons of geometrically linear and non-linear PFDD and APFM with atomistics are carried out in the context of the simulation of (i) lattice distortion and stress in the dislocation core and slip plane regions, and (ii) the Peierls stress, in Al and Au. Generally speaking, only geometrically non-linear APFM (PFDD) predicts lattice distortion in the dislocation core and slip-plane regions in agreement with atomistics. In comparison to APFM and atomistics, the Peierls stress of screw dislocations in Al is over-predicted by GPN/PFDD by about an order of magnitude, most likely due the much narrower and "stiffer" GPN/PFDD-based dislocation core.

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Title: Modeling Grain Boundary Anisotropy-Driven Microstructural Evolution with Arbitrary Grain Orientation and Plastic Deformation Boundary Driven

Author(s): *Josep Maria Ribot, *UCCS* ; Brandon Runnels, *Department of Mechanical and Aerospace Engineering University of Colorado, Colorado Springs*.

The aim of this work is to increase the understanding of polycristalline materials by determining the effect of anisotropic grain boundary energy on dissipative deformation mechanisms, using realistic models for the boundary energy between conjoining grains with varying lattice orientations in a polycrystalline sample. Using data dynamically computed for boundary energy from the model developed in previous works [1] at the atomistic scale for FCC and BCC materials, a phase field model has been implemented that incorporates these atomistically determined properties with elastic finite elements. In this work we consider simplified 2d polycrystalline metals. The boundary energy model is coupled with Cahn-Hilliard kinetics, using diffusive (finite width) boundaries. With the model for computing the grain boundaries evolution, several loading conditions have been applied (axial stress, pure shear, combined stress patterns). After unloading the sample, some deformation persists due to the grain boundary relocation to less energetic configuration during the loading cycle, indicating the effect of anisotropy on grain boundary mediated elastoplasticity. Creep deformation has also been studied by applying several loading-unloading cycles to the sample. The results of the present work gives physical insight into the effect of grain boundary anisotropy in the context of grain boundary engineering, looking towards producing digitally micro-designed materials with tailored properties for high performance applications. [1] B. Runnels, I. J. Beyerlein, S. Conti, and M. Ortiz, “A relaxation method for the energy and morphology of grain boundaries and interfaces,” Journal of the Mechanics and Physics of Solids, vol. 94, pp. 388 – 408, 2016.

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Title: A Physics-Based Reduced-Order Model for the Dynamic and Post-Buckling Behavior of Tensegrity Structures and Metamaterials

Author(s): *Julian Rimoli, *Georgia Tech*.

Traditional approaches for modeling the behavior of tensegrity structures have their origin either on form-finding applications or on the desire to capture their quasi-static behavior. As such, they generally assume that (i) bars are perfectly rigid, (ii) cables are linear elastic, and (iii) bars experience pure compression and strings pure tension. In addition, a common design constraint is to assume that the structure would fail whenever any of its bars reaches the corresponding Euler buckling load. In reality, these assumptions tend to break down in the presence of dynamic events. In this work, we develop a physics-based reduced-order model to study aspects related to the dynamic and nonlinear response of tensegrity-based structures. With very few degrees of freedom, our model captures their buckling and post-buckling behavior as well as their dynamic response. We then adopt our model to show how, under dynamic events, buckling of individual members of a tensegrity structure does not necessarily imply structural failure. Finally, we show how through successive reflection operations it is possible to architecture a 3D tensegrity metamaterial, and analyze its response to impacts. Our research suggests that efficient structural design of impact-tolerant tensegrity structures and metamaterials could be achieved by exploiting rather than avoiding the buckling behavior of its compression members.

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Title: Optimization-Based Anisotropic Mesh-Polynomial Adaptation for High-Order Methods

Author(s): *Nicolas Ringue, Siva Nadarajah, *McGill University*.

Adaptive unstructured high-order methods form a promising framework to improve the computational efficiency, robustness and reliability of Computational Fluid Dynamics (CFD) algorithms. Since industrial CFD applications often result in complex flow solutions, error estimation and control are essential to assess the validity of numerical approximations. Furthermore, as they rely on arbitrary discretizations of space and time, the efficiency and accuracy of the numerical methods can potentially be optimized for a given flow simulation. The use of optimization related concepts has been increasingly considered to guide mesh adaptation, from the use of local merit functions [1] to the global mesh size optimization via a surrogate error model [2]. Following these recent developments, we propose a general unifying framework for anisotropic hp-adaptation of high-order discontinuous Galerkin finite element discretizations for compressible flow simulation. Based on the concept of mesh-metric duality [3], a Riemannian metric field and polynomial degree distribution are used to form a continuous mesh representation and formulate an optimization problem. Using the sensitivities of a goal-oriented (adjoint-based) error estimate with respect to both metric and polynomial degree, our method solves for a distribution of degrees of freedom minimizing the global error on a target quantity of interest, such as aerodynamic coefficients. This results in an optimal hp-mesh tailored to yield the most accurate prediction of a functional of the flow solution at a given computational cost. The proposed approach features reduced dependence on the initial mesh, as well as on a priori user input compared to established adjoint-based adaptive methods. It provides a unifying framework where adaptation choices such as isotropic/anisotropic, h-/p-refinement/coarsening do not only rely on local arbitrary measures of the solution anisotropy and smoothness, but rather where a globally optimal distribution of degrees of freedom is directly sought to minimize the error in the chosen quantity of interest. References: [1] M. Ceze and K. J. Fidkowski. Anisotropic hp-adaptation framework for functional prediction. AIAA Journal, 51(2):pp. 492–509, 2013. [2] M. Yano and D. L. Darmofal. An optimization-based framework for anisotropic simplex mesh adap- tation. Journal of Computational Physics, 231:pp. 7626–7649, 2012. [3] A. Loseille and F. Alauzet. Continuous mesh framework part I: well-posed continuous interpolation error. SIAM Journal on Numerical Analysis, 49(1):pp. 38–60, 2011.

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Title: An Extended Finite Element Model for Studying Shear Dilation in a Pressurized Medium

Author(s): *Endrina Rivas, Robert Gracie, *University of Waterloo*.

Hydraulic fracturing is used in oil and gas production to optimize the reservoir conductivity so that wellbore production can be increased. The changes in the stress state in the naturally fractured medium surrounding the hydraulically activated volume can cause shearing of the natural fractures. Shearing of discontinuities in rocks is accompanied by shear dilation, or normal displacement that occurs along fracture surfaces due to surface roughness of the joints. Shear dilation can be a major source of permeability enhancement from hydraulic fracturing stimulation [1]. A two-dimensional model of shear dilation along a network of natural fractures is implemented in the extended finite element method (XFEM). XFEM has been used by various researchers to model hydraulic fracturing, including contact and friction [2], and fracture propagation [3], but has not yet been developed to model shear dilation. As hydraulic fracture models advance, this capability is required to assess the permeability enhancement generated by shear dilation during the stimulation. Contact, friction, and dilation are modeled along the crack surface, and are satisfied by imposing non-linear constraints along the fracture surfaces. The locations of discontinuities in the medium are known a priori, which represent the pre-existing natural fractures in a rock. A node-to-node contact algorithm is implemented under the assumption of small displacements, such that the contact search is limited to predefined node pairs. Using this model, the development of shear dilation along a network of natural fractures is simulated and accuracy and stability of the results will be discussed. This will be used to analyze the shear dilation developed due to hydraulic fracturing stimulation. References: [1] Zhou, L., Su, X., Hou, Z., Lu, Y., & Gou, Y. (2016). Numerical investigation of the hydromechanical response of a natural fracture during fluid injection using an efficient sequential coupling model. Environmental Earth Sciences, 75(18), 1263. [2] Dolbow, J., Moës, N., & Belytschko, T. (2001). An extended finite element method for modeling crack growth with frictional contact. Computer Methods in Applied Mechanics and Engineering, 190(51–52), 6825–6846. [3] Gordeliy, E., & Peirce, A. (2013). Coupling schemes for modeling hydraulic fracture propagation using the XFEM. Computer Methods in Applied Mechanics and Engineering, 253, 305–322.

14th U.S. National Congress on Computational Mechanics
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Title: Use of the Conformal Decomposition Finite Element Method for Coupled Electrochemical-Mechanical Simulations of Lithium-Ion Battery Electrodes

Author(s): *Scott Roberts, Hector Mendoza, Bradley Trembacki, Mark Ferraro, Victor Brunini, David Noble, *Sandia National Laboratories*.

The Conformal Decomposition Finite Element Method (CDFEM) is an algorithm for creating a dynamic, multi-material computational mesh that is sharply conformal to material interfaces. While its original intent was for moving interface fluids problems, it has recently become particularly useful for generating static meshes for complex material domains. An example of this is lithium-ion battery electrode microstructures, which are comprised of a percolated network of non-spherical solid particles, conductive polymer binder, and liquid electrolyte. Three-dimensional reconstructions of these microstructures are created using imaging techniques (such as X-ray computed tomography), and conformal meshes are created directly using CDFEM, skipping the difficult step of manually creating a mesh. In this talk we discuss verification of this CDFEM-based approach for microstructure meshing, using a number of geometric and simple physical metrics for quantifying the error associated with mesh resolution, domain size, and mesh quality. We also relate these simple metrics to the results of fully-coupled electrochemical-mechanical simulations of battery discharge, commenting on how well electrode performance can be captured through simple metrics. Additionally, we discuss the role of the polymeric binder on electrode properties and explore various options for binder placement. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. Unclassified Unlimited Release: SAND2017-1974 A

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Title: Large Amplitude Aeroelastic Oscillations of a Cantilever with Structural and Aerodynamic Nonlinearities: Theory and Wind Tunnel Test

Author(s): *Brandon Robinson, Leandro Jose Rocha da Costa, Abhijit Sarkar, *Carleton university*; Dominique Poirel, *Royal Military College of Canada*; Chris Pettit, *United States Naval Academy*; Mohammad Khalil, *Sandia National Laboratories*.

A flexible airfoil which undergoes edgewise bending, flapwise bending, torsion and base rotation is modelled as a nonlinear coupled aeroelastic system with nonlinearities in the structure and aerodynamic moment. The equations of motion of the airfoil are given by a system of three coupled, nonlinear partial differential equations (PDEs) and an ordinary differential equation (ODE). The solution to the system of PDEs and ODE is obtained by adopting a Galerkin projection scheme, leading to a coupled nonlinear ODE system, integrated numerically. The structural equations are derived using Hamilton's Principle by da Costa. The aerodynamic lift acting in the edgewise direction is modelled as linear while the nonlinear aerodynamic moment is modelled empirically as polynomials of structural displacements and velocities, using wind tunnel data obtained from experiments at the Royal Military College of Canada. Previous endeavours into the analysis of the dynamics of this coupled, nonlinear aeroelastic system have focussed on the nonlinear effects that stem from the inherent geometric nonlinearities of the structure itself, opting to model the aerodynamic loads according to linear theories (quasi-steady and unsteady aerodynamics). Prior experiments such as those documented in Poirel et al. for single-degree-of-freedom (pitch) and for two-degree-of-freedom (pitch and plunge) respectively, analyse the nonlinear aerodynamics from wind-tunnel data at a transitional Reynolds number, though they have assumed a simpler, linear model for the structure itself. The use of wind-tunnel data herein and its application to a continuous system circumvents some of the physical and mathematical complexities that are associated with deriving an analytical nonlinear model of the aerodynamic forces, while still allowing for a more comprehensive analysis of the dynamical phenomena that arise from the interaction of the nonlinear aerodynamics and structural dynamics.

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Title: Pressure Induced Damage of Pulmonary Artery: Mechanical Parameters Estimation

Author(s): Marissa Grobbel, Hailu Getachew, Yuheng Wang, Laura Nye, Seungik Baek, *Sara Roccabianca, *Michigan State University*.

Pulmonary hypertension (PH) is associated with elevated pulmonary arterial pressure. One of known features of human PH is a large increase of caliber, more than 50% increase in young patients. In this study, we investigate the damage mechanism in the arterial wall associated with over-pressurization due to PH. The hypothesis tested here is that increased arterial pressure can alone significantly damage the vessel wall. We use an experimental in vitro porcine model to estimate the mechanical behavior of the arterial wall before and after the damage occurs. Further, we suggest that increased transmural pressure associated with PH can induce irreversible damage in the pulmonary artery wall contributing to the remodeling of the vessel. Two main branches of a porcine PA are dissected. One is then prepared for pressure-dimeter test and the other is prepared for histology (control). The pressure-diameter protocol consists of 6 phases (a to f) of five inflation-deflation cycles for the pressure ranges as follows: (a) preconditioning, 0-30 mmHg; homeostatic (b) and (c) 0-50 mmHg (two times); over-pressurization (d) and (e) 0-100 mmHg (two times); (f) homeostatic again, 0-50 mmHg. Then, the tested specimen and the control are prepared for histology. The stains used are, Verhoeff-Van Gieson (VVG) to identify the elastin, and Masson's Tri-Chrome (MTC) to identify collagen and smooth muscle cells (SMC). To separate elastic fibers, SMC, and collagen fibers based on hue, saturation, and lightness thresholding we used custom MATLAB routines. The area fraction for elastin is evaluated as the ratio between pixels identified as elastin, i.e. black in a VVG stain, and the total pixels of tissue identified in the slide. The area fraction for SMC, and collagen fibers from the MTC stained slides is evaluated in the same manner. To describe the measured biaxial behavior we employ the "four-fiber family" constitutive description introduced by [1] incorporating the model with the area fractions of constituents, as described above. Briefly, three of the six pressure dimeter-protocols described before are employed to find two sets of best-fit material parameters for the constitutive relation. Specifically, protocols (b-c) and (f) are used to describe the mechanical behavior before and after pressure-induced damage, respectively. Best-fit values were determined by minimizing the error between theoretically predicted and experimentally measured pressures via a nonlinear least squares regression [2]. References: [1] Baek, S. et al. J. Biomech. Eng. 128.1: 142-149, 2006. [2] Roccabianca, S. et al. J.R. Soc. Interface 11.97: 20140397, 2014.

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Title: A Bayesian Analysis of Rheological Models for the Simulation of Turbidity Currents

Author(s): *Fernando Rochinha, Henrique Costa, Zio Souleymane, Gabriel Guerra, Alvaro Coutinho, *COPPE-UFRJ*.

Numerical models can help to push forward the knowledge about complex dynamic physical systems. The modern approach to doing that involves detailed mathematical models. Turbidity currents are a kind of particle-laden flows that represent a very complex natural phenomenon. In a simple way, they are turbulent driven flows generated between fluids with small density differences carrying particles. They also are one mechanism responsible for the deposition of sediments on the seabed. A detailed understanding of this phenomenon, including uncertainties, may offer new insight to help geologists to understand reservoir formation, a strategic knowledge in oil exploration. We present a finite element residual-based variational multiscale formulation applied to the numerical simulation of particle-laden flows in a Eulerian-Eulerian framework. Thus, the mathematical model results from the incompressible Navier-Stokes equation combined with an advection-diffusion transport equation. When sediment concentrations are high enough, rheological empirical laws close the model, describing how sediment concentrations influence the mixture viscosity. The aim of this work is to investigate the effects on the flow dynamics of some these empirical laws. We use two configurations for numerical experiments. The first is a lock-exchange configuration in a tank and the second employs a channel with sustained current. Both numerical experiments are inspired in complex laboratory tests. We show how turbulent structures and quantities of interest, such as sediment deposition, are affected by the different empirical rheological laws. Moreover, we employ a Bayesian framework to validate the employed hypothesis and introduce a stochastic error term for taking into account the modeling error.

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Title: Extended Variational Quasicontinuum Methodology for Modelling of Crack Propagation in Discrete Lattice Systems

Author(s): *Ondrej Rokos, Ron H.J. Peerlings, *Eindhoven University of Technology*; Jan Zeman, *Czech Technical University in Prague*; Lars A.A. Beex, *Universite du Luxembourg*.

Lattice models can be successfully used for modelling materials with discrete micro- or meso-structures, mainly because they can relatively easily incorporate non-localities, complex constitutive laws, and large fibre deformations or reorientations. Typical examples of such materials are 3D-printed structures, woven textiles, paper, foams, or concrete. The accuracy, generality, and simplicity of discrete models come usually at the expense of excessive computational cost. This is due to the multi-scale nature of engineering problems, which require large number of interactions as the application scale is often much larger compared to the size of individual links. The Quasicontinuum (QC) methodology, introduced by Tadmor et al. [1], was developed to overcome this kind of limitation for conservative atomistic systems at the nano-scale. Recently, extensions towards models with dissipative interactions at the meso-scale have been developed, first based on the Coleman-Noll procedure in [2], and later based on the variational theory of energetic rate-independent systems in [3]. QC, as a concurrent multiscale method, is especially suitable for modelling of damage, fracture, and crack propagation in discrete materials, mainly due to the fact that the dissipative mechanisms and nonlocalities matter most in a relatively small fracture process zone near the crack tip. Elsewhere, interpolation and coarse-graining can be used. In this presentation, the necessary extensions of variational QC towards an effective modelling of crack propagation in discrete mesoscopic systems are discussed, including the following concepts: (i) definition and geometrical description of cracks, (ii) introduction of partition-of-unity-based concepts and enrichment of the displacement interpolation, (iii) generalization of summation rule to accurately sample the incremental energy of the extended system, (iv) reconstruction of energy quantities upon mesh refinement and coarsening, and (iv) development of effective and robust mesh refinement and coarsening strategy. The efficiency and performance of the method thus obtained is demonstrated on a number of test examples. References [1] E. B. Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. Philosophical Magazine A, 73(6):1529–1563, (1996). [2] L. A. A. Beex, R. H. J. Peerlings, and M. G. D. Geers. A multiscale quasicontinuum method for dissipative lattice models and discrete networks. Journal of the Mechanics and Physics of Solids, 64:154–169, (2014). [3] O. Rokos, L.A.A. Beex, J. Zeman, R.H.J. Peerlings. A variational formulation of dissipative quasicontinuum methods. International Journal of Solids and Structures, 102-103:214–229, (2016).

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Title: New Numerical Methods for the Efficient Coupling of Nonlinear Beams and Continua

Author(s): *Ignacio Romero, *IMDEA Materials*.

A long standing problem in numerical methods for structural mechanics concerns the effective coupling of structural models (beams, shells, etc.) and continua. This issue is of practical importance because, in order to optimize computational resources, finite element models of complex mechanical systems very often need to combine reduced-dimension bodies and continua. At their interfaces, special coupling techniques have to be applied to reconcile their kinematics. In particular, beams and shells have translational and rotational degrees of freedom, and linking their kinematics to continuum bodies (which only have translational degrees of freedom) demands special strategies. In the past, transitions finite elements have been proposed for 2D linear analyses [1,2], but also multi-point constraints, and iterative techniques [3]. In this work we propose an new strategy to consistently couple the kinematics of beams and continua, based on a variational principle-at the continuum level-that imposes weakly compatibility. The discretization of such principle leads to mixed or penalty formulations that effectively link to two models, for two- or three-dimensional problems, with linear and nonlinear kinematics. In the talk, the theory behind the new variational principles will be presented, and illustrative examples will be provided. [1] K S Surana. Isoparametric elements for cross-sectional properties and stress analysis of beams. International Journal for Numerical Methods in Engi- neering, 14:475–497, 1979. [2] H S Kim and S M Hong. Formulation of transition elements for the analysis of coupled wall structures. Computers & Structures, pages 333–344, 1995. [3] P Mata, A H Barbat, and S Oller. Two-scale approach for the nonlinear dy- namic analysis of RC structures with local non-prismatic parts. Engineering Structures, 30(12):3667–3680, December 2008.

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Title: A Direct Flux Reconstruction Formulation for Advection-Diffusion Problems on Simplex Elements

Author(s): *Joshua Romero, Freddie Witherden, Antony Jameson, *Stanford University*.

The direct flux reconstruction (DFR) scheme is a high-order numerical method which is an alternative realization of the flux reconstruction (FR) approach. In 1D, the DFR scheme has been shown to be equivalent to the FR variant of the nodal discontinuous Galerkin (DG) scheme [1]. This equivalence in 1D leads naturally to equivalence of the DFR scheme in 2D and 3D on quadrilateral and hexahedral elements through the use of tensor products. In this presentation, an extension of the DFR approach to triangular and tetrahedral elements for advection and advection-diffusion problems is described. The scheme for advection problems is generated by combining aspects of the SD-RT variant of the spectral difference (SD) scheme for triangles developed by May et. al. [2], with modifications motivated by characteristics of the DFR scheme in one dimension, namely the use of a flux divergence which is one order higher than that used for the solution reconstruction. To extend the application of the scheme to diffusive fluxes, a novel approach to computing the solution gradients is developed which enables computation of the gradients via direct application of the procedure to compute the flux divergence. The talk will discuss these developments in detail, contrasting with existing flux reconstruction approaches on simplices. Furthermore, the results of numerical experiments to characterize the numerical performance and accuracy of the scheme will be presented. [1] Romero, J., Kartikey Asthana, and Antony Jameson. "A Simplified Formulation of the Flux Reconstruction Method." Journal of Scientific Computing 67.1 (2016): 351-374. [2] May, G., and J. Schöberl. "Analysis of a spectral difference scheme with flux interpolation on raviart-thomas elements." Aachen Institute for Advanced Study in Computational Engineering Science (2010).

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Title: Time and Space Adaptivity in Turbidity Current Simulation

Author(s): *Andre Rossa, Alvaro Coutinho, Jose Camata, *Federal University of Rio de Janeiro*.

In this work, we investigate the role of particles sedimentation and the influence of particle settling on the flow dynamics of turbidity (or density) currents with special attention to the lock-exchange problem. Turbidity currents is a class of geological flow phenomenon with multiple scales in time and space and have a leading role in the formation of hydrocarbon reservoirs, which is known to host a large amount of Brazilian reserves (Camata et al., 2013). Turbidity currents can change the physical shape of the sea floor by eroding and/or depositing soil over large areas creating underwater geological formations with oil and gas reservoirs. Sedimentation effects are modeled considering a given constant settling velocity of the grains current. At the end of each time-step, the mass flux of particles at the domain's bottom is computed and its integration along time results into boundary displacements which are used to update the mesh arising an Arbitrary Lagrangian Eulerian (ALE) coupled sedimentation model. For such a class of multiphysics and multiscale problems, space and time adaptability may be mandatory to solve a real scenario simulation. With this goal in mind we have been used libMesh FEM library for simulating sedimentation problems found in turbidity currents considering feedback theory-based time-step control and adaptive mesh refinement and coarsening (AMR/C). The incompressible Navier-Stokes and transport equations are solved using the Residual-based Variational Multiscale Method (RB-VMS) (Lins et al., 2009). To the transport problem, we add a discontinuity-capturing term. Good agreement was obtained for deposit profiles in a monodisperse particle-driven current with available experimental (from de Rooij and Dalziel, 2001) and computational references. Results suggest that libMesh is a versatile numerical tool for investigating the interactions between turbidity currents and seafloor topography, helping fundamental sedimentological studies for hydrocarbon reservoirs characterization.

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Title: Combined Segregated-Fully Coupled Hydro-Mechanical Cracking of Concrete Using XFEM in 3D

Author(s): *Simon-Nicolas Roth, Azzeddine Soulaïmani, *École de Technologie Supérieure*; Pierre Léger, *École Polytechnique de Montréal*.

In industries such as dam engineering and exploration of natural gas from hydrocarbon-rich shale formations, multiphysical phenomena such as fluid flow simulation during cracks evolution should be modeled correctly. This type of flow may be linear or non-linear. If a linear flow is used, a fully coupled system of equations can be solved without adding much complexity to the nonlinear cracking problem. For more complex flows such as non-Newtonian fluid flow, turbulent flow in a crack, inclusion of geometrical features like drains in dams, the flow may present severe nonlinearities. Solving the nonlinear cracking problem together with the nonlinear flow features several difficulties. Because the presence of cracks subjected to hydraulic pressures in plain concrete structures is a major concern for their durability, serviceability and stability, the method presented in this work is particularly targeting applications in dam engineering. Flow laws in cracks depends on various parameters such as aperture, roughness, tortuosity and Reynold's numbers. Depending on these parameters, the formulation of the hydraulic problem leads to a system of nonlinear equations. The inclusion of drains, with nearby very strong hydraulic gradients, makes it necessary to have different (multi-physics) finite element models; one with a hydraulic mesh and one with a mechanical mesh. Therefore, the hydraulic and mechanical subproblems are solved using a partitioned procedure, as they have different resolution requirements. Hence, a second fully automated hydraulic mesh is generated on the crack surface. Because their computational domains have non-matching discrete interfaces, a key aspect is the transfer of the structural crack apertures to the hydraulic mesh, and the transfer of the hydraulic pressures to the mechanical problem by respecting the applied load equilibrium. In this work, the proposed approach for modeling nonplanar 3D cracks in plain concete structures uses a continuous damage model (CDM) with transition to cohesive XFEM model. The XFEM formulation makes possible the computation of the crack aperture as well as the application of pressures on the crack surfaces for simulation of hydraulic fracture initiation and propagation. During the first stages of crack evolution, a fully coupled hydro-mechanical model, including nonlinear permeability linked with damage evolution, is used. The validation examples presented in this work are limited to dam engineering related problems, however the proposed method can be used for simulation of other type of hydraulic fracturing problems.

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Title: Approximating the Fluctuations in Random Heterogeneous Problems

Author(s): *Pierre-Loïk Rothé, *Navier/CERMICS (ENPC)*; Frédéric Legoll, *Navier (ENPC)*.

Computing the homogenized properties of random materials is often very expensive. The full-field approach consists in considering a large RVE, and solving the equilibrium problem on that RVE, submitted to e.g. periodic boundary conditions. Besides the (averaged) behavior of the material response on large space scales (which is given by its homogenized limit), another question of interest is to understand how much this response fluctuates around its coarse approximation. More generally, we aim at understanding which parameters of the distribution of the material coefficients affect the distribution of the response, and whether it is possible to compute that latter distribution without resorting to a brute force Monte Carlo approach. In this talk, this question will be addressed both from a theoretical and a numerical standpoints. We will show that, using the standard corrector function of random homogenization, we are able to compute a tensor which completely governs the fluctuations of the response. Joint work with F. Legoll.

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Title: SiGran: A Virtual Laboratory for Geotechnical Applications

Author(s): *Varvara Roubtsova, Mohamed Chekired, *IREQ (Hydro-Quebec)*.

SiGran is a highly parallel software dedicated to numerical modeling of geotechnical phenomena such as soil liquefaction, internal and external erosion, among others. This software has been developed at Hydro-Quebec's research institute (IREQ). The main concepts of this virtual laboratory are multi-physics and multi-scale simulations. Failure, at the micro level, of the interaction between particles when water flows into the pore channels can result in the collapse of structures such as dams. The Discrete Element Method (DEM), which simulates particle motion based on Newton's laws, and Marker-And-Cell (MAC), which models the transient viscous fluid flows by solving the Navier-Stokes equations, are used at the micro level. Particle influence on water flow was taken into account by utilizing special non-slipping conditions. Conversely, the force acting on a particle due to water flow was calculated by integrating the pressure field and viscous stresses around the particle. Smoothed Particle Hydrodynamics (SPH) method was used at the macro level to resolve the system of governing equations for continuum mechanics. The material behavior equation is based on the results of simulations carried out at a micro level. The possibility of combining three methods (DEM, MAC and SPH) will be discussed. The OpenCL framework was used in order to achieve a high level of data parallelism on NVIDIA Graphics Processing Units (GPU) based on Tesla High Performance Computing (HPC) hardware. Ongoing comparison of results obtained by simulation with theoretical and experimental data was carried out during development of the virtual laboratory. The most interesting results include the study of particles interaction in viscous fluids, testing permeability, liquefaction phenomenon, among others.

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Title: Modelling Microfluidic Sample Traps to Optimize Trapping and Culture of Ex Vivo Biological Samples

Author(s): *Nassim Rousset, Frédéric Monet, *Polytechnique Montréal*; Thomas Gervais, *Polytechnique Montréal, CRCHUM*.

Microfluidic Sample Traps (MSTs) are a widely used class of microfluidic device that moves samples through a main channel and into wells or recesses adjacent to that channel with applied flow rates. The simplicity of MST design makes it a convenient solution for simultaneously transporting, individually trapping, imaging and releasing large quantities of samples. However, for biological research applications, certain design parameter constraints must be considered to optimize ex vivo biological sample viability. This viability can be negatively affected by extreme shear stresses and nutrient depletion through sample trapping, culture and treatment exposure. Trapping stability, trapping time, shear stress and sample metabolism in MSTs can be optimized by using the finite element method, design parameter sweeps and phase diagrams. Studying hydrodynamic and diffusion-reaction effects in an MST are key to understand the effect of operating a device with flow rates or periodical medium change on the viability of ex vivo biological samples. Ultimately, combining results from analytical models and nearly 15,000 numerical simulations into condensed phase diagrams leads to optimal design parameter ranges for a spherical tissue of a given diameter ($d<500\mu m$). The simplest and closest to optimal trap shape for a MST is a slightly shallow square prism of a given side w and height $h\approx0.9w$; where $w\approx2d$. These dimensions ensure that ex vivo biological samples are not subject to damaging shear stresses while remaining trapped in an MST. Additionally, ensuring optimal sample metabolism for 24 hours without perfusion requires an available medium volume per trap that is 100× the tissue volume. The latter simulation results were validated by comparing experimental procedure in various published articles to the predicted viability times by this numerical model. This work demonstrates the specific biological application of MSTs; however, the hydrodynamic results are also valid for inorganic samples and the numerical method can also be applied to help design any microfluidic device with a well-defined parameter space. More fundamentally, combining the finite element method, parameter sweeps and phase diagrams is an adaptable method that enables studying a design parameter space with many degrees of freedom.

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Title: A Feasible Minimum Energy State Method for Constrained, Multi-Disciplinary Topology Optimization Problems

Author(s): *Willem Roux, *LSTC*.

This new topology design method is for very large vehicle models being designed for a combination of frequency analysis, linear statics, and explicit dynamic load cases. For simple topology optimization a gradient descent is sufficient, but extensions are required for the constrained, multi-disciplinary problems under consideration. In this method a gradient descent vector is sourced from the various analysis disciplines, while the multi-disciplinary constraints are satisfied by descending to a minimum energy state of the structure that satisfies these constraints. So in this approach a subproblem is solved to computed the feasible minimum energy state, and this computation of the energy state is done using a design of experiments approach as used in other optimization disciplines. Examples are given to clarify the utility of this approach.

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Title: Electro- and Magneto-Mechanical Coupling and Instabilities in Dielectric Elastomers and Magnetorheological Elastomers

Author(s): *Stephan Rudykh, Artemii Goshkoderia, *Technion*.

Dielectric elastomers (DEs) can achieve large deformations when excited by an electric field. This ability makes DEs promising candidates for muscle like actuators for soft robotics applications. Motivated by potential enhancement of the electromechanically coupling in DEs, microstructured DEs have attracted significant attention. In this work, we study the electromechanical behavior of DE composites with circular and elliptical inclusions embedded in a matrix; DE composites are subjected to finite strains and external electrostatic stimuli. We analyze the role of the material properties, and geometrical parameters, and applied electromechanical loadings on the effective properties of the DE composites. We specifically focus on the instability phenomenon in the DE composites with periodically distributed inclusions embedded in soft matrix. The corresponding unit cells are constructed and analyzed by means of a finite element based numerical tool. The applied electromechanical loadings are imposed in terms of periodic boundary conditions. To determine the onset of electromechanical instabilities, a general stability condition is utilized [1, 2]. We identify the unstable domains in terms of material and microstructure parameters and electromechanical loading. We show that electric field can either stabilize or destabilize the DE composites depending on the microstructure [3]. Due to some mathematical similarities, the numerical procedure can be applied to magnetorheological elastomers, thus, allowing to determine the magneto-mechanical behavior and stability of the magnetoactive composite materials. References: [1] Rudykh S., Bhattacharya K. and deBotton G.: Multiscale instabilities in soft heterogeneous dielectric elastomers. Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 470(20130618), 2014 [2] Rudykh S., and deBotton G., Stability of Anisotropic Electroactive Polymers with Application to Layered Media. Z. Angew. Math. Phys.(ZAMP), 62, 1131–1142 (2011) [3] E. Galipaeu, S. Rudykh, G. deBotton and P. Ponte-Castaneda, Magnetoactive elastomers with periodic and random microstructures. International Journal of Solids and Structures, 51, 3012–3024 (2014)

14th U.S. National Congress on Computational Mechanics
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Title: Multiscale Fracture Analysis of Materials with Periodic Microstructure

Author(s): *Michael Ryvkin, *Tel Aviv University*.

The main tool for reducing the computational cost of solving fracture problems is provided by multiscale methods which, as a rule, are based on the decomposition of the analysis domain into coarse scale and fine scale subdomains. However, in some cases the fine scale domain which is required for the adequate modeling of the fracture phenomenon remains relatively large and its analysis still presents a numerical challenge. A method is suggested to overcome this difficulty in the case of heterogeneous periodic composite material. The fine scale domain is viewed as an assemblage of perfectly bonded repetitive cells. The analysis of non-periodic stress field in this domain is reduced to the analysis of single representative cell by means of the discrete Fourier transform. As a result, the analysis of large periodic region is replaced analytically by the analysis of single repetitive cell in the transform space. It may be viewed as using a periodic fine mesh and further analyzing the one repetitive module. The analysis of repetitive cell is performed several times in order to carry out the inverse transform. Examples of employing such procedure can be found in [1,2]. The method is illustrated with an analysis of three-point bending crack problem for periodically voided two-dimensional material which is anisotropic at a macroscale. References: [1] Ryvkin, M. and Hadar, O. ”Employing of the discrete Fourier transform for evaluation of crack-tip field in periodic materials”, International Journal of Engineering Science, 2015, 86, 10-19. [2] Ryvkin, M., Hadar, O. and Kucherov, L. "Multiscale analysis of composites with periodic microstructure" (submitted).

14th U.S. National Congress on Computational Mechanics
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Title: Effect of Discretization and Stochastic Material Distribution on Crack Initiation in Peridynamics

Author(s): *Martin Rädel, Christian Willberg, Jochen Schmidt, *German Aerospace Center (DLR)*.

The simulation of the structural behavior and particularly damage response is a key instrument for the development of lightweight structures as required in aerospace engineering or wind rotor blade development. The prediction of damage initiation and propagation in main structural elements as well as their adhesive bonds is a challenging task, even for state-of-the-art numerical procedures, such as the finite element method (FEM). The peridynamic theory presents a promising approach for these requirements. It is a non-local theory which takes long-range forces between material points into account. The theory assumes that a material point interacts with all its neighboring particles within a finite radius. The formulation of its governing equations is based on integral equations, which are valid everywhere - in a non-disturbed material region as well as in the vicinity or directly at a discontinuity such as a crack. Damage is directly incorporated in the material response ([1],[2]). Additionally, the mesh-free peridynamic implementation in the open-source code Peridigm promises to overcome the mesh dependency problems currently present in FEM or extended FEM (XFEM) methods. In the current publication, the effect of a varying discretization and the stochastic distribution of material properties is investigated and compared to other fracture mechanical methods based on a tensile test on an epoxy specimen. It is examined if a more realistic representation of the stiffness distribution can lead to improved results regarding crack initiation and propagation compared to the standard models. These normally assume perfect symmetry. The applied framework and the underlying theory and its numerical implementation are introduced. [1] S. A. Silling (2000) Reformulation of elasticity theory for discontinuities and long-range forces. Journal of the Mechanics and Physics of Solids, 48, 175-209. [2] F. Bobaru, J. T. Foster, P. H. Geubelle, S. A. Silling (2017) Handbook of Peridynamic Modeling., CRC Press, Boca Raton

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Title: On the In-Vivo Function of the Heart Valve Leaflet: Insights into Tissue-Interstitial Cell Biomechanical Coupling

Author(s): Chung-Hao Lee, *University of Oklahoma*; Will Zhang, *Michael Sacks, *The University of Texas at Austin*.

The proper choice of the reference configuration, and the determination of its resulting pre-stresses of biological systems, is a fundamental question in computational biomechanics. The incorporation of such an important piece of information is essential to facilitating realistic biomechanical simulations of the heart valves by making a connection to tissue homeostasis. Thus, this study aims to develop an inverse finite element modeling framework for characterizing the in vivo tissue properties and estimating the functional stresses of the heart valves, by incorporating the previously quantified pre-strains due to the change of the reference configurations [1]. Specifically, a two-step simulation procedure is developed, in which a simulation of the dimensional changes is first performed to recover the stress-free configuration at the in vitro reference configuration, and then an expansion simulation is carried out based on such a stree-free configuration to its in vivo functional valve geometry followed by the inverse modeling of heart valve function over cardiac cycles. Tissue mechanical properties are determined by minimizing the valve surface geometry between the experimental data and simulated one. Our results show that the pre-stretches (1.323 and 1.346 in the circumferential and radial directions, respectively) result in fairly isotropic pre-stresses of ~20-30 kPa that are relatively small (<10%) compared to the estimated in vivo functional tissue stresses. These pre-stress results further indicate that the long toe-region of the valve tissue stress-strain behavior, typically observed in vitro [2], is completely absorbed by the pre-strain. This implies that the elastin fiber network is primarily responsible for the pre-strains, whereas collagen fibers subsequently bear the majority of in vivo physiological loading. Our novel results allow to make an important connection between the in vivo functional state and the in vitro reference configuration, which will be beneficial to defining an appropriate form of the strain energy function for realistic biomechanical modeling of the heart valves. We are currently investigating the effects of surgical repair by implanted an annuloplasty ring on the alterations of organ- and tissue-level mechanical loading/deformation. Integration of such information within a biomechanical modeling framework will ultimately facilitate the development of simulation-guided management of valvular heart disease with improved long-term surgical outcomes. References: [1] Amini et al. (2012) Ann Biomed Eng 40: 1455-1467. [2] Grashow et al. (2006) Ann Biomed Eng 34: 1509-1518.

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14th U.S. National Congress on Computational Mechanics
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Title: Computational Homogenization Accounting for Size Effect via Interface Elasticity at the Micro-Scale

Author(s): *Saba Saeb, Paul Steinmann, *Erlangen-Nuremberg University*; Ali Javili, *Bilkent University*.

The objective of this presentation is to establish a computational homogenization framework to model the behavior of heterogeneous materials in which the influence of interfaces at the micro-scale is taken into account. The term “interface” refers to a zero-thickness model that represents the finite thickness “interphase” between the different phases of the micro-structure. Therefore, the interface is essentially a two-dimensional manifold embedded in a three-dimensional space. The interface effect is particularly important at the microscopic level and often dominates the mechanics of nano-structures due to the increasing area-to-volume ratio at small scales. Hence, it is of significant importance to account for interfaces at the micro-scale. We show that an immediate consequence of including the interface at the micro-scale is the introduction of a length-scale into first-order computational homogenization. Therefore, the proposed interface-enhanced computational homogenization framework captures size effects in the material response that are missing in classical computational homogenization. In this contribution, the interface does not allow for a displacement jump across the interface and hence, is only valid for coherent interfaces. However, the traction jump, which is mainly due to the elasticity along the interface, is permitted. Central to computational homogenization is the Hill-Mandel condition which ensures the incremental energy equivalence between the macro- and the micro-scale. A generalized version of the Hill-Mandel condition is presented that accounts for the presence of the interface at the micro-scale. Accordingly, suitable boundary conditions to satisfy the Hill-Mandel condition are derived. Moreover, extended average theorems, in particular average deformation gradient and average stress theorems, are employed to relate the macroscopic quantities to their microscopic counterparts. The computational aspects of the proposed framework using the finite element method are detailed. Finally, the influences of different boundary conditions on the overall response of the micro-problem with different sizes, geometries and interface properties are discussed through presenting several numerical examples.

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Title: A Bayesian Framework for the Estimation of Regional Methane Fluxes

Author(s): *Cosmin Safta, Ray Bambha, Hope Michelsen, *Sandia National Laboratories*.

We present a hierarchical Bayesian framework to estimate surface methane fluxes based on atmospheric concentration measurements and a Lagrangian transport model (Weather Research and Forecasting and Stochastic Time-Inverted Lagrangian Transport model). Structural errors in the transport model are estimated with the help of co-emitted trace species with well-defined decay rates. We conduct the analyses at regional scales that are based on similar geographical and meteorological conditions. For regions where data are informative, we further refine flux estimates by emissions sector.

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Title: A Numerical Study of Branching and Stability of Solutions to Three-Dimensional Martensitic Phase Transformations Using Gradient-Regularized, Non-Convex, Finite Strain Elasticity

Author(s): *Koki Sagiyama, Krishna Garikipati, *University of Michigan*; Shiva Rudraraju, *University of Wisconsin*.

In the setting of continuum elasticity, phase transformations involving martensitic variants are modeled by a free energy density function that is non-convex in strain space. Here we aim for microstructures in which martensitic variants form twin structures. We adopt an existing mathematical model in which we regularize the non-convex free energy density function by higher-order gradient terms at finite strain and derive boundary value problems via the standard variational argument applied to the corresponding total free energy, inspired by Toupin's theory of gradient elasticity. These gradient terms are to preclude existence of arbitrarily fine microstructures, while still allowing for existence of multiple solution branches corresponding to local minima of the total free energy; these are classified as metastable solution branches. The goal of this work is to numerically obtain these metastable solutions in three dimensions. To our knowledge this is the first work that studies branching of solutions and observes twin structures in three-dimensional diffuse-interface problems based on a non-convex density function regularized by strain gradient terms.

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Title: The Importance of Mechano-Electrical Feedback and Inertia in Cardiac Electromechanics

Author(s): *Francisco Sahli Costabal, Ellen Kuhl, *Stanford University*; Felipe A. Concha, Daniel E. Hurtado, *Pontificia Universidad Catolica de Chile*.

In the past years, a number cardiac electromechanics models have been developed to better understand the excitation-contraction behavior of the heart. However, there is no agreement on whether inertial forces play a role in this system. In this study, we assess the influence of mass in electromechanical simulations, using a fully coupled finite element model. We include the effect of mechano-electrical feedback via stretch activated currents. We compare five different models: electrophysiology, electromechanics, electromechanics with mechano-electrical feedback, electromechanics with mass, and electromechanics with mass and mechano- electrical feedback. We simulate normal conduction to study conduction velocity and spiral waves to study fibrillation. During normal conduction, mass in conjunction with mechano-electrical feedback increased the conduction velocity by 8.12% in comparison to the plain electrophysiology case. During the generation of a spiral wave, mass and mechano-electrical feedback generated secondary wavefronts, which were not present in any other model. These secondary wavefronts were initiated in tensile stretch regions that induced electrical currents. We expect that this study will help the research community to better understand the importance of mechanoelectrical feedback and inertia in cardiac electromechanics.

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Title: Theoretical and Computational Modeling of Lipid Membranes: Effects of Elastic Bending and In-Plane Viscous Flow

Author(s): *Amaresh Sahu, Kranthi Mandadapu, *UC Berkeley*; Yannick Omar, Roger Sauer, *RWTH Aachen*.

Biological membranes comprised of lipids and proteins make up the boundary of the cell, as well as the boundaries of internal organelles such as the nucleus, endoplasmic reticulum, and Golgi complex. While lipid membranes and their interactions with proteins play an important role in many cellular processes, lipid membranes also pose a unique modeling challenge because they bend elastically out-of-plane but behave in-plane as a two-dimensional fluid. We present the theory of irreversible thermodynamics for arbitrarily curved lipid membranes, which describes the coupling between elastic bending and the irreversible processes of intra-membrane lipid flow, intra-membrane phase transitions, and protein binding and diffusion. We employ this framework in the linear regime to develop the governing equations of motion, as well as appropriate boundary conditions. We then discuss the dynamics of lipid membranes, using these equations of motion, using a newly developed Augmented Lagrangian-Eulerian (ALE) finite method formulation. The ALE formulation allows us to study the coupling between elastic bending and viscous in-plane flow, especially in the context of large deformations and non-axisymmetric membrane geometries.

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Title: Multi-Component Topology Optimization: Historical Developments and Continuous Relaxation

Author(s): Yuqing Zhou, *Kazuhiro Saitou, *University of Michigan*.

Topology optimization is a computational synthesis for structures by optimally distributing a material(s) within a prescribed design domain. Since the geometry is represented non-parametrically, it facilitates innovative designs through the exploration of arbitrary shapes. However, such unconstrained exploration also tends to generate structures difficult to manufacture. One of the primary reasons, which surprisingly has rarely been discussed, is that conventional topology optimization assumes the optimized structure is made as a single-piece. To relax this assumption, the multi-component topology optimization (MCTO), an evolution of conventional monolithic topology optimization, simultaneously optimizes not only the overall structural topology, but also the component partitioning. Preliminary results show that manufacturing constraints previously applied to monolithic topology optimization gain new interpretations when applied to multi-component assemblies, which unlocks richer design space for topology exploration of structural designs with economical manufacturing. The presentation will first introduce the advent of the MCTO research in 1990s, followed by a summary of historical developments of this topic in our group since early 2000s. We first modeled the MCTO problem in discrete formulations, therefore all solved by non-gradient methods (e.g. multi-objective genetic algorithms). The presentation will then focus on our recent continuous relaxation of the MCTO in a SIMP-like formulation with additional variables specifying fractional component membership [Zhou and Saitou, 2017a]. The continuous formulation, for the first time*, enabled the use of an efficient gradient method to solve the MCTO, which dramatically improved the computational efficiency, and opened up new opportunities for future developments. Applications of the MCTO to sheet metal structures considering stamping die cost [Zhou and Saitou, 2017a], and to additive manufacturing structures considering printer build volume, enclosed voids, and support materials [Zhou and Saitou, 2017b] will be discussed to demonstrate the continuous relaxation. The advantages of the MCTO over conventional monolithic topology optimization in economical manufacturing will be presented. Opportunities for future research will also be discussed in the end of the presentation. Zhou, Y. and Saitou, K., 2017(a), Gradient Multi-Component Topology Optimization of Sheet Metal Structures with Stamping Die Cost Manufacturing Constraint, WCSMO12 (accepted) Zhou, Y. and Saitou, K., 2017(b), Multi-Component Topology Optimization of Additive Manufacturing Structures with Printer Build Volume and Enclosed Void Manufacturing Constraints, IDETC2017 (submitted) *In the scope of all previous works in the multi-component topology optimization from Algorithmic Synthesis Laboratory (ASL) at University of Michigan.

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Title: A Coupled Numerical Model for Discrete Fractures in Deformable Geothermal Reservoirs

Author(s): *Saeed Salimzadeh, *Technical University of Denmar*; Maiya Medetbekova, Hamidreza M. Nick, *Technical University of Denmark*.

In geothermal systems, the contraction of the rock matrix due to the heat extraction alters the contact tractions on the existing fractures. The contact stress alteration changes the local aperture distribution, and that results in creation of conductive paths between the injector and the producer. The conductive paths can reduce the lifetime of a geothermal system by preventing the cold fluid from accessing the heat stored in the bulk reservoir (MIT Report, 2006). The extent of the aperture variation also depends on the heterogeneity in the aperture distribution (Guo et al, 2016). The reduction of contact tractions on the fractures may increase the chance for sliding of the fractures and shear propagation of fractures. Radial Jet Drilling (RJD) is a novel stimulation technique that uses the power of fluids (water and/or acids) to drill lateral holes through tubing. RJD is currently investigated within the H2020 SURE project (Novel Productivity Enhancement Concept for a Sustainable Utilization of a Geothermal Resource) to assess its stimulation performance and potential productivity increase. In this work, the effect of thermal volume contraction on the aperture variation in a fractured geothermal system is investigated. A fully coupled thermo-hydro-mechanical (THM) model is developed using finite element method. Discrete fractures are modelled as 2D surfaces within 3D rock matrix. The model has been implemented into an object-oriented software and validated against several benchmark examples. The contact tractions between fractures surfaces have been computed using a robust contact model modified for THM effects. Development of short-circuits within fractures plane during lifetime of a geothermal system are observed in the simulations. Three modal stress intensity factors are computed to investigate the propagation of the fractures. The utility of the RJDs in further accessing the bulk volume of the hot rock, and reducing the local aperture variation is investigated and results will be presented. Keywords: Thermal fracturing, thermo-poroelasticity, stress intensity factors, geothermal systems, aperture variation References MIT Report: The future of geothermal energy: impact of enhanced geothermal systems (EGS) on the United States in the 21st century[R]. America: Massachusetts Institute of Technology, 2006. Guo B., Fu P., Hao Y., Peters C.A., Carrigan C.R. 2016. Thermal drawdown-induced flow channeling in a single fracture in EGS, Geothermics, 61: 46-62.

14th U.S. National Congress on Computational Mechanics
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Title: A Hybridized Discontinuous Galerkin Method for Fully Nonlinear Irrotational Serre-Green-Naghdi Model

Author(s): *Ali Samii, Clint Dawson, *University of Texas at Austin*.

The high nonlinearity and dispersive properties of the water waves near the coast has resulted in the development of different mathematical models to simulate the wave motion in these regions. Although, the fluid motion in such regions is a three dimensional process, the Boussinesq wave theory considers a polynomial distribution for the velocity field in the vertical direction and reduces the problem to a two dimensional description. Here, we first recall the well-known shallowness, nonlinearity, and topography parameters, which are used to describe the dominant features in our problem. Next, we compare some wave models based on their assumptions on the magnitude of these parameters or based on the highest power of each parameter included in the model. Next, we consider solving a recent version of the Serre-Green-Naghdi equation using a combination of hybridized DG (HDG) and local DG (LDG) methods. We first decompose the equation to hyperbolic and dispersive parts. The hyperbolic part of the problem is basically the nonlinear shallow water equation. The dispersive part requires a system of equations to be solved implicitly in each time step. Since HDG results in a system of equations with less number of degrees of freedom and smaller bandwidth compared to the other DG variants, it is a good choice for performing this implicit solve step. On the other hand, solving this system requires estimation of higher order derivatives of the velocity vector. To this end, we need a method with explicit definition of the numerical fluxes. Hence, we use local DG to estimate these derivatives. Finally, we solve a set of numerical examples to verify and validate our numerical results. We demonstrate optimal convergence of the proposed technique and a good match between the numerical results and experimental data.

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Title: A Conservative Streamline Method Suitable For Complex Reservoir Flow Simulations

Author(s): Gerritsen Margot, Anthony Kovscek, *Luiz Sampaio, *Stanford University*; Marco Thiele, *Stanford University / Streamsim Technologies*.

The Finite Volume Method is widely used in reservoir simulation. Its formulation is inherently conservative, mimicking the fundamental physical laws. On the other hand, Finite Volume discretization is not accurate for strongly advective flows in multiple dimensions, as grid orientation effects and numerical diffusion usually cause large computational errors. The Streamline Method provides an alternative approach. It uses paths following the velocity vector as a support for the discretization, producing a set of uncoupled, one dimensional problems. Each of these independent problems can be more easily and efficiently solved, as special treatments can explore particular properties of 1D advection. To combine the strenghts of both methods, reservoir simulations commonly use a hybrid approach in which the relevant equations are each solved with the most suitable method and the solution fields are mapped back and forth from a Finite Volume grid to the set of streamlines. In this hybrid approach, the conservation property is usually violated during the mapping step. This is a concern for simulation of flows with strong volume changes, as is the case of many multiphase, multiphysics reservoir flows. To overcome this, we developed a streamline formulation that is mass conservative down to machine precision. In this work, we motivate the new formulation, and show its derivation as well as some verification tests.

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Title: Symplectic HDG Methods for Wave Propagation Phenomena

Author(s): Bernardo Cockburn, *Manuel Sanchez, *University of Minnesota*; Ngoc Nguyen, Jaime Peraire, *MIT*.

We devise the first symplectic Hybridizable Discontinuous Galerkin (HDG) methods for the acoustic wave equation. We discretize in space by using an HDG scheme and in time by using symplectic, diagonally implicit and explicit partitioned Runge-Kutta methods. The key characteristic of the semi-discrete scheme is it preserves the Hamiltonian structure of the wave equation, which combined with symplectic time integrators guarantees the conservation of the energy. We obtain optimal approximations of order $k+1$ in the L^{2}-norm when polynomials of degree $k\geq0$ and Runge-Kutta formulae of order $k+1$ are used. In addition, by means of post-processing techniques and augmenting the order of the Runge-Kutta method to $k+2$, we obtain superconvergent approximations of order $k+2$ in the L^2 norm for the displacement and velocity. We provide numerical examples corroborating these convergence properties as well as depicting the conservative features of the methods.

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Title: PDE-Constrained Optimization Framework for the Design of Heterogeneous Elastic Acoustic Cloaks

Author(s): *Clay Sanders, Wilkins Aquino , *Duke University*; Timothy Walsh, *Sandia National Laboratories*.

We present a PDE-constrained optimization framework for the design of heterogeneous elastic materials for acoustic cloaking applications. We achieve optimal distributions of linear-elastic, isotropic materials which allow solid scatterers to be cloaked from harmonic acoustic excitation. The complex design task is posed as a PDE-constrained optimization problem: the optimal distribution of elastic material in a cylindrical scatterer is selected to minimize the residual between a pressure field from an unobstructed spreading wave in fluid and the scattered field produced by the solid inclusion. Design variables are formulated in two schemes, either enforced as an interpolation between two material phases or allowed to vary continuously. The nonlinear constrained optimization problem is solved using a reduced-space adjoint formulation, leveraging the differentiability of the objective and the set of linear constraints, a coupled acoustic-structural Helmholtz equation system, for efficient gradient calculations. The optimal distribution designs-- neutrally-buoyant cylinders featuring radial variation in elastic bulk modulus--effectively eliminate reflections from incident acoustic pressure. These designed distribution patterns achieve cloaking behavior for both individual frequencies and extended frequency bandwidths. The presented design framework may be extended to other generalized geometries and physically realized with novel functionally graded or composite elastic materials. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL850000.

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Title: CAD-Based Patient-Specific Vascular NURBS Modeling for Isogeometric Analysis

Author(s): Benjamin Urick, *The University of Texas*; *Travis Sanders, Thomas J.R. Hughes, *The University of Texas at Austin*; Shaolie Hossain, *Texas Heart Institute*; Jessica Zhang, *Carnegie Mellon University*.

Patient-specific vascular modeling involves three main steps: (1) image processing, (2) analysis suitable model generation, and (3) computational analysis. Analysis suitable model generation currently suffers from difficulties and complications, which often necessitate manual intervention and geometry approximations. Because the modeling pipeline spans multiple disciplines, domains, and expertise, the benefits of integrating a computer-aided design (CAD) component for the geometric modeling tasks has been largely overlooked. In this work, a new CAD-integrated vascular modeling framework is presented, streamlining the production of solid NURBS (non-uniform rational B-spline) vascular models for isogeometric analysis (IGA). In general, geometries used in finite element analyses can be categorized into two classes: user-defined geometries and geometries derived from images. Historically, CAD technologies have been employed by designers to generate models from scratch, whereas image-based geometries are typically handled by purpose-built software because of the added difficulty involved in sampling data. CAD software, however, is generally agnostic to source and should be seen as a powerful, robust, and rigorously tested geometry library that is useful for any algorithm requiring geometry manipulation and visualization. CAD systems also offer specific advantages for vascular modeling including speed, accuracy, interoperability, user-friendliness, and feature creation such as stent insertion. We implemented a template-based [1] vascular model generation algorithm in the CAD software Rhinoceros 3D® (Rhino) with Grasshopper 3D® (Grasshopper). First, a triangulated surface mesh and corresponding centerlines are extracted from the segmented 3D image stack and provided as inputs to the algorithm. Next, sampling frames are distributed along the centerlines of the artery tree. Special attention is given to regions near arterial bifurcations to ensure the sampling frames do not intersect. Next, the triangulated surface mesh is sampled, forming a polyline on each sampling frame. Then, a NURBS curve is interpolated through each polyline and the curves are lofted along the centerline to form the lumen boundary. Finally, introducing a radial direction to the parameterization completes the solid model. IGA of blood flow is performed on the resulting hexahedral NURBS mesh to compute quantities of interest such as wall shear stress. To instantiate the claim that complex geometries can be handled with this approach, example applications are presented including the Circle of Willis in a mouse and a porcine coronary artery tree. References: [1] Y. Zhang, Y. Bazilevs, S. Goswami, C.L. Bajaj, T.J.R. Hughes, Patient-specific vascular NURBS modeling for isogeometric analysis of blood flow, Comput. Methods Appl. Mech. Eng. 196 (2007) 2943–2959. doi:10.1016/j.cma.2007.02.009.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Bayesian Model Selection in Continuous Model Domain Using Automatic Relevance Determination with Applications to Nonlinear Aeroelasticity

Author(s): *Rimple Sandhu, Abhijit Sarkar, *Carleton university*; Chris Pettit, *United States Naval Academy*; Mohammad Khalil, *Sandia National Laboratories*; Dominique Poirel, *Royal Military College of Canada*.

Bayesian model selection provides a robust tool to compare several plausible models of nonlinear dynamical systems by assimilating noisy measurements of the system response while accounting for modelling uncertainties. Bayesian model selection using non-asymptotic evidence estimator powered by Markov Chain Monte Carlo(MCMC) sampling has been used to estimate the posterior model probabilities [1, 2]. The optimal model chosen through the Bayesian approach provides the best tradeoff between the average data-fitting capability and model complexity. The reliability of Bayesian model selection results depends on a 'good' candidate model set and carefully chosen prior distributions of model parameters with limited knowledge. However, it is well-known that Bayesian model selection results are misleading when the prior distributions are chosen arbitrarily. Automatic relevance determination (ARD) complements Bayesian model selection by providing a mathematical apparatus to find the optimal model nested under an overly complicated model without having to propose the candidate nested models and assign prior distributions to model parameters with limited knowledge. The prior distributions for model parameters with limited knowledge are assumed to be zero-mean Gaussian with unknown variances, being the hyper-parameters. These hyper-parameters govern the relevance of the corresponding model parameters to the system dynamics. The optimal hyper-parameter values are estimated by maximizing model evidence. The superfluous model parameters are pruned away during evidence maximization by their corresponding hyper-parameters, thereby making them irrelevant for prediction purposes. Hence, ARD operates by parameterizing the prior distributions for selected model parameters which in turn converts the model selection problem from a discrete model domain to a continuos model space. The optimal nested model selected using ARD approach embodies the concept of Occams razor by producing posterior distributions of the model parameters that occupy a parsimonious subset of the model space. References [1] R. Sandhu, D. Poirel, C. Pettit, M. Khalil and A. Sarkar, Bayesian inference of nonlinear unsteady aerodynamics from aeroelastic limit cycle oscillations. Journal of Computational Physics. 2016. [2] Sandhu, R., Pettit, C., Khalil, M., Poirel, D. and Sarkar, A., Bayesian model selection using automatic relevance determination for nonlinear dynamical systems, Journal of Computer Methods in Applied Mechanics and Engineering, accepted, 2017.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: An Integrated Approach for Fluid-Structure Interaction: Uncertainty Quantification, Bayesian Inference, Scalable Algorithms for High Performance Computing and Wind Tunnel Testing

Author(s): Rimple Sandhu, Leandro Jose Rocha da Costa, Brandon Robinson, Anton Matachniouk, Sandip Chajjed, Philippe Bisaillon, Ajit Desai, *Abhijit Sarkar, *Carleton University*; Mohammad Khalil, *Sandia National Laboratories*; Chris Pettit, *United States Naval Academy*; Dominique Poirel, *Royal Military College of Canada*.

We report a rational statistical framework for credible and efficient analysis and prediction in fluid-structure interaction (FSI) by using high performance computing (HPC). The Bayesian statistical method offers a natural framework to handle complex interplay between uncertainty (e.g. structural defects) and nonlinearity (e.g. large structural deflection, flow separation) in FSI systems by reconciling numerical simulations by observational data for credible and realistic predictions. Wind tunnel testing feeds Bayesian analysis by providing observational data required for model selection and calibration. For efficient uncertainty quantification and inference of the fluid and structural systems, multi-level domain decomposition method based iterative solvers are developed which will have the potential to exhibit scalable performance by leveraging massive concurrency of next generation HPC systems. Using wind tunnel tests, the proposed framework is applied to investigate a new type of limit cycle oscillation (induced from flow separation) of flexible lifting surfaces at transitional Reynolds numbers.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A C^0 Non-Local Model of Hydraulic Fracturing

Author(s): *Erfan Sarvaramini, Robert Gracie, Maurice Dusseault , *University of Waterloo*.

Hydraulic fracturing simulation in highly heterogeneous and naturally fractured formations leads to the development of a complex fracture network with a priori unknown fracture propagation paths. The ability to model this complexity is crucial to the design of a hydraulic fracturing process and mitigation of the potential environmental risks of the reservoir containment breach and induced seismicity. The application of non-local models to predict and understand the behavior of fluid-driven fractures in heterogeneous formations has gained increasing attention in recent years. Traditional non-local FEA models require C^1 continuity of the trial and test functions, which complicates their implementations, compared to the traditional C^0 FE interpolants. Here, a new C^0 non-local model to simulate the initiation and propagation of the hydraulic fractures will be presented. The C^0 continuity requirement is achieved through a reformulation of traditional non-local models. The plastic softening damage is combined with the classic Biot poroelastic theory to account for the hydraulic-mechanical coupling behavior. The proposed model is implemented using the Galerkin finite element method. The predictor-corrector radial return algorithm combined with a consistent tangent operator for the gradient based plasticity is used to quantify the evolution of the localized plasticity. The performance of proposed methodology is tested by considering examples of hydraulic fracture propagation calculations.

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14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Mechanical Properties of Human Ascending Aorta Using Biaxial Tensile Testing

Author(s): *Samaneh Sattari, Katherine Olsen, Taisyia Sigaeva, Jehangir J. Appoo, Elena S. Di Martino, *University of Calgary*.

Ascending thoracic aortic aneurysms are pathological enlargements of the vessel at the level of thoracic ascending aorta. They are generally asymptomatic; however, when they become symptomatic, they often present in catastrophic fashion. Therefore, there is urgency to determine which aneurysms are benign and which need elective surgery. Understanding the biomechanical properties and the characteristics of aortic wall can improve the accuracy of computational analysis and provide improved indications for elective surgery patient selection. Therefore, we investigated the mechanical properties of aneurysmal tissues in this study and compared them with structural information from histology. Fresh samples were collected from 5 patients undergoing ascending aortic replacement. Biaxial tensile test, which stretches sample in both circumferential and axial directions simultaneously, was used with different five tension ratios including 1:1, 1:075, 1:0.5, 0.5:1, 0.75:1 to find mechanical properties of tissues. The tissue was assumed as an incompressible, homogenous, hyperelastic material undergoing finite quasi-static isothermal deformation. Under these assumptions, we can consider a strain energy function, which defines the elastic response of the sample. The strain-stress curves for each patient for all five protocols were fitted to a Fung-like constitutive model with three parameters (Hyperfit) [1]. This model characterizes behavior differences between two loading directions. On the other hand, histology images of these tissues were used to quantify changes in constituents of aorta. The elastin fragmentation was graded from 0 (normal) to 3 (severe). Our results showed that there is a non-linear relationship between stress and strain. The experimental data were fitted very well to the Fung model with R2 in the range of 0.83- 0.97. The aneurysmal aortic tissues were stiffer in the circumferential than in the axial direction in 4 out of 5 patients. There was also a relationship between stiffness and material constants. Circumferentially stiffer tissues had higher material parameter a1 compared to a2. The constant a3 which indicates the cross talk between circumferential and axial direction, was negligible. Moreover, the anisotropy indices obtained from the material constants were more than 0.85 in 3 out of 5 patients, indicating a high level of anisotropy. The histology images of these 3 patients (with higher anisotropy) showed elastin fragmentation with grade 1 or 2 while elastin abnormality for the 2 patients with lower anisotropy indices were of grade 3, indicating a higher degree of disorganization due to loss of extracellular tissue structure. [1] Fung et al.; Pseudoelasticity of arteries and the choice of its mathematical expression; the American Physical Society (1979).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Liquid-Solid Contact: Algorithms for Sticking and Sliding

Author(s): *Roger Sauer, *RWTH Aachen University*.

In contrast to classical solid-solid contact, liquid-solid contact is governed by the contact line, where a contact angle can form and undergo hysteresis. Liquid-solid contact therefore requires additional contact algorithms that capture the contact state at the contact line. Altogether four contact algorithms are required in order to describe the general contact behavior between solids and liquids: frictionless surface contact, frictional surface contact, frictionless line contact [1] and frictional line contact [2]. For the latter, a new predictor-corrector algorithm is presented that enforces the contact conditions at the contact line and thus distinguishes between the states of advancing, pinning and receding contact lines. All four algorithms are discretized within a monolithic finite element formulation. Several numerical examples are presented focusing on rolling and sliding droplets. For quasi-static droplets, the interior medium follows a hydro-static pressure relation that does not require discretization. For dynamic droplets, the interior fluid flow is accounted for through the incompressible Navier-Stokes equations. [1] R.A. Sauer (2014), "Stabilized finite element formulations for liquid membranes and their application to droplet contact", Int. J. Numer. Meth. Fluids, 75(7):519-545 [2] R.A. Sauer (2016), "A frictional sliding algorithm for liquid droplets", Comput. Mech., 58(6):937-956

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Fast Multipole Method for Poroelastodynamics

Author(s): *Martin Schanz, *Graz University of Technology*.

Wave propagation phenomena occur in reality often in semi-infinite two-phase (porous) regions. It is well known that such problems can be handled well with the poroelastodynamic Boundary Element Method (BEM). But, it is also well known that the BEM with its dense matrices becomes prohibitive with respect to storage and computing time. This is especially true for poroelastodynamics, where in the best case four degrees of freedom (dofs) per node are required. For partial saturated porous materials even five dofs are necessary. Additionally to this efficiency problem also numerical problems occur due to the different physical nature of the matrix entries, which vary over several orders of magnitude. Last, the fundamental solution of poroelastodynamics is computationally expensive. Here, the fast multipole method (FMM) is applied to reduce the complexity of the poroelastodynamic BEM to an almost linear order. Due to the complicated fundamental solutions a black-box type FMM is preferable. The proposed black-box FMM-BEM uses the Chebyshev interpolation-based FMM. This, firstly, reduces the number of evaluations of the computationally expensive fundamental solution significantly. Second, for large problems, the storage requirement of the FMM-BEM operators is almost linear. A significant compression is achieved using the SVD to compress the M2L-operators. Numerical tests show as well asymptotically an almost linear behavior with respect to the CPU-time. It must be remarked that the iterative solver works only if the problem is transformed to dimensionless variables. The presented results show that the proposed FMM can be adjusted such that the convergence rates of the standard BEM can be obtained.

14th U.S. National Congress on Computational Mechanics
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Title: Coupling Bio-Physical Tumor Models With Diffeomorphic Image Registration

Author(s): *Klaudius Scheufele, Miriam Mehl, *University of Stuttgart*; Amir Gholaminejad, Andreas Mang, George Biros, *University of Texas at Austin*.

Gliomas are a class of brain tumors, among them the most common malignant form of gliomas is Gliobalstoma (GBM) that exceeds in its mortality rate beyond other types of brain tumors. Despite of significant advances in medical treatment, the median life expectancy of patients with GBM is less than 12 months, with only 5% of these patients surviving five years after diagnosis. Quantifying the volume and other morphological characteristics of a tumor is an important indicator of the disease progression, as well as the efficacy of the therapy. We aim at identifying initial conditions and characterizing parameters of tumor growth based on a combination of image registration and parameter estimation (by solving an inverse tumor growth problem). This allows us to predict future tumor growth as a basis for actual modeical decisions on the further patient-specific treatment. The presented work focuses on optimization of the overall coupled system tightly connecting both parts as a decisive step to actual applicability in a clinical context. Both, image registration and tumor growth are inverse problems. Whereas the image registration maps the patient image with tumor to a standardized atlas brain with tumor, the inverse tumor solver inverts for initial conditions and growth parameters from a given atlas brain with tumor. The registration step becomes neccessary as the healthy patient brain without tumor is inaccessible in practice. We combine them to a PDE constrained optimization formulation in which the image similarity functional is coupled to a bio-physical model. The glioma growth is modeled by a reaction-diffusion partial differential equation. This setup can be utilized to solve a parameter estimation problem for a model of low-grade glioma growth. Here, the goal is to estimate the spatial distribution of tumor concentration, as well as the magnitude of anisotropic tumor diffusion or the rate of cell proliferation. We consider a semi-monolithic coupling and solve the PDE constrained optimization in an optimize then discretize fashion with the standard adjoint approach. To this end, we make use of different quasi-Newton and inexact Gauß-Newton variants to solve the non-linear system of PDEs. Typically, clinical real brain data is of high resolution, thus providing simulation results in pertinent time requires for highly scalable solvers and application on massively parallel HPC systems. We present a highly scalable and efficient simulation environment to solve this challenging coupled multi-component problem.

14th U.S. National Congress on Computational Mechanics
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Title: Amorphous Silica: From Molecular Dynamics to the Continuum

Author(s): *William Schill, Stefanie Heyden, Michael Ortiz, *Caltech*.

Glass is attractive for high velocity impact resistant applications because of its low density, high strength, volume expansion following fracture and energy dissipation due to densification. At the present the engineering community lacks continuum models of Silica glass that characterize all of these effects, thereby limiting efforts to probe the ultimate utility of this glass in application. We model a representative volume element of the glass using molecular dynamics, probing densification, pressure-shear coupling, and the viscoelastic response. Specifically, our molecular dynamics calculations reveal anomalous decreasing shear yield stress behavior of this amorphous solid with increasing pressure. We then formulate a constitutive law to capture this behavior borrowing techniques from the Cam clay theories of soil mechanics. The anomalous shear behavior requires special attention to properly treat while passing to the continuum. We hope that this combination of efforts constitutes a novel approach to modeling amorphous Silica and, more generally, provides a new view of coupling atomistic modeling of amorphous solids to the continuum.

14th U.S. National Congress on Computational Mechanics
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Title: Adaptivity through Localization in Model Reduction for Parabolic Problems

Author(s): Mario Ohlberger, Stephan Rave, *Felix Schindler, *University of Münster*.

We present recent advances in the context of the localized reduced basis multi-scale method for parametric scalar elliptic [1] and parabolic [2] multi-scale problems with possibly heterogeneous diffusion coefficients. In particular we present localized error control for the full approximation error (including discretization and model reduction error) and various aspects of adaptivity, based on this localized error control. [1]: Ohlberger, M. and Schindler, F. Error Control for the Localized Reduced Basis Multiscale Method with Adaptive On-Line Enrichment. SIAM J. Sci. Comput., Vol. 37, pp. A2865-A2895, (2015). [2]: Ohlberger, M. and Rave, S. and Schindler, F. True Error Control for the Localized Reduced Basis Method for Parabolic Problems. arXiv [math.NA], 1606.09216, (2016), https://arxiv.org/abs/1606.09216.

14th U.S. National Congress on Computational Mechanics
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Title: A New Particle-In-Cell Technique for Reducing Noise

Author(s): Chenfanfu Jiang, *University of Pennsylvania*; *Craig Schroeder, *University of California, Riverside*; Joseph Teran, *University of California, Los Angeles*.

We present a new technique for transferring momentum and velocity between particles and grid with Particle-In-Cell (PIC) calculations which we call Affine-Particle-In-Cell (APIC). APIC represents particle velocities as locally affine, rather than locally constant as in traditional PIC. We show that this representation allows APIC to conserve linear and angular momentum across transfers while also dramatically reducing numerical diffusion usually associated with PIC. Notably, conservation is achieved with lumped mass, as opposed to the more commonly used Fluid Implicit Particle (FLIP) transfers which require a 'full' mass matrix for exact conservation. Furthermore, unlike FLIP, APIC retains a filtering property of the original PIC and thus does not accumulate velocity modes on particles as FLIP does. In particular, we demonstrate that APIC does not experience velocity noise that is characteristic of FLIP in a number of Material Point Method (MPM) hyperelasticity calculations. Lastly, we demonstrate that when combined with the midpoint rule for implicit update of grid momentum that linear and angular momentum are exactly conserved.

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Title: U-Splines: Application as a Basis for Isogeometric Analysis

Author(s): *Michael Scott, Zhihui Zou, *Brigham Young University*; Derek Thomas, Kevin Tew, *Coreform LLC*; Michael Borden, *North Carolina State University*.

U-splines are a new spline description which alleviates the challenges associated with building analysis-suitable smooth bases over unstructured grids. U-spline basis functions are positive, form a partition of unity, and are locally linearly independent and overcome the analysis-suitability mesh constraints required by T-splines (including near extraordinary points and T-junctions). In this talk, the application of U-splines as a basis for isogeometric analysis will be discussed.

14th U.S. National Congress on Computational Mechanics
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Title: A Variational Multiscale Method for Dynamic Viscoelastic Solid Mechanics

Author(s): *Guglielmo Scovazzi, Nabil Abboud, Oriol Colomés, *Duke University*; Xianyi Zeng, *University of Texas El Paso*.

We develop a dynamic version of the variational multiscale (D-VMS) stabilization for nearly/fully incompressible solid dynamics simulations of viscoelastic materials. The constitutive models considered here are based on Prony series expansions, which are rather common in the practice of finite element simulations, especially in industrial/commercial applications. Our method is based on a mixed formulation, in which the momentum equation is complemented by a pressure equation in rate form. The unknown pressure, displacement and velocity are approximated with piecewise linear, continuous finite element functions. In order to prevent spurious oscillations, the pressure equation is augmented with a stabilization operator specifically designed for viscoelastic problems, in that it depends on the viscoelastic dissipation. We demonstrate the robustness, stability, and accuracy properties of the proposed method with extensive numerical tests in the case of linear and finite deformations. Time permitting, we will also discuss the use of this proposed methodology in the context of failure mechanics.

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14th U.S. National Congress on Computational Mechanics
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Title: Electromechanical Peridynamic Modeling of Deformation and Damage Sensing in Polymer Bonded Explosive Materials

Author(s): Naveen Prakash, *Gary Seidel, *Virginia Tech*.

Peridynamics, a recently developed non-local theory of continuum mechanics is being favored over traditional finite element based methods to model complex phenomena in solids such as the crack initiation, branching and propagation. The non-local nature of peridynamic equations allows one to overcome issues such as mesh dependent results and ill conditioned matrices. Peridynamic equations have also been extended to model multiphysics problems such as heat diffusion, coupled thermomechanics, fluid flow, corrosion among others. In this work, a computational electromechanical framework based on peridynamics is used to investigate the strain and damage sensing properties of nanocomposite bonded explosive materials (NCBX). Polymer or plastic bonded explosives are a type of energetic materials consisting of explosive grains dispersed in a polymer binder. These complex materials are susceptible to damage in a low velocity impact event during transportation and handling, which can weaken the material in addition to the possibility of accidental ignition. Therefore, it is important to monitor in real time, the structural health of the material for safe transportation and handling. It is proposed that dispersing carbon nanotubes within the binder phase will allow for in-situ structural health monitoring owing to the unique piezoresistive properties of nanocomposites. The peridynamics computational framework allows in capturing key deformation mechanisms like interface debonding and granular fracture which are important in assessing the piezoresistive response in the damage regime. The role of many parameters such as impact velocity, grain conductivity, and interface properties among others are investigated in detail through peridynamic simulations. The computational results presented in this work indicate that there is promise for in - situ monitoring of granular energetic materials based on the piezoresistive properties of nanocomposites which may prove to be advantageous over current methods.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Multiscale Optimization Using Generalized Mortar Methods

Author(s): *Daniel Seidl, Bart van Bloemen Waanders, Tim Wildey, *Sandia National Laboratories*.

A long-standing challenge in computational science and engineering is the accurate and efficient modeling of physical systems with interactions that occur over multiple length and/or time scales. Representative example problems include prediction of flow through an oil reservoir, weather forecasting, and characterization of additive manufacturing processes. Furthermore, when such systems represent constraints in inverse and optimal control problems their solution may be required hundreds to thousands of times over the course of the optimization algorithm. In such problems, direct numerical simulation is often prohibitive and thus a multitude of numerical methods that utilize a coarse scale approximation of the underlying fine scale physics have been developed. In this talk we present a variant of the multiscale mortar method where the macro-scale discretization is defined in terms of the trace of the basis functions on the interior skeleton of a macro-scale finite element mesh. Each macro-element contains a localized and independent representation of the fine scale problem physics, i.e. mesh, model fidelity, time integration scheme, etc can vary within each macro-element. Given the coarse-scale solution as Dirichlet data, these local fine-scale problems are solved independently leading to an efficient parallel implementation that can leverage emerging heterogeneous computational architectures. The coarse scale residual and Jacobian are defined in terms of the local Dirichlet-to-Neumann map projected into the mortar space. We show that this approach has a consistent space-time variational formulation and is thus amenable to adjoint-based sensitivity calculations. Given an objective function, we formulate and solve a multi-scale adjoint problem leading to an efficient and accurate calculation of its gradient. We demonstrate our approach on an inverse problem with a variable density of sensor measurements and the optimal control of a nonlinear transient thermoelastic problem that emulates additive manufacturing. Our results will be compared to those obtained using only a coarse-scale model and to those obtained using direct numerical simulation.

14th U.S. National Congress on Computational Mechanics
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Title: Peridynamic Models for Anisotropic Media

Author(s): *Pablo Seleson, *Oak Ridge National Laboratory*; Jeremy Trageser, *George Washington University*; Max Gunzburger, *Florida State University*.

Peridynamics is a nonlocal reformulation of classical continuum mechanics, suitable for material failure and damage simulation. Originally, this nonlocal theory was presented as a bond-based theory, for which the material response of an isotropic medium is limited by a fixed Poisson's ratio. To overcome this limitation, the state-based theory was developed. Applications in peridynamics to date cover a wide range of engineering problems; however, the majority of those applications employ isotropic material models. Only recently, a limited number of anisotropic peridynamic models were developed. In this talk, we will first survey the different classes of anisotropic material models in classical linear elasticity, and we will present anisotropic peridynamic models. We will show a classification and a hierarchy of those models, and we will discuss their relation to classical elastic models, as well as restrictions arising from a bond-based interaction assumption.

14th U.S. National Congress on Computational Mechanics
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Title: Mesh-Free Particle Modeling of Multiphase Granular Continuum

Author(s): *Ahmad Shakibaeinia, *Polytechnique Montreal*.

A mesh-free particle method for continuum-based modelling of dry and immersed (multiphase) granular flows is presented. The multiphase system of the granular matter and the ambient fluid is treated as a multi-density multi-viscosity continuum, in which the viscous behaviour of the granular phase is predicted using a regularized viscoplastic rheological model with a pressure-dependent yield criterion. The numerical technique is based on a weakly-compressible Moving Particle Semi-implicit (WC-MPS) method and μ(I) rheological model. The required techniques for numerical approximation of the effective viscosity, effective pressure, and shear stress divergence are introduced. The model is validated and evaluated for wide range of granular regimes (free-fall, grain inertia, viscous regimes) for flow-driven and gravity-driven granular benchmarks such as granular collapse and sediment scouring. The comparison of the results with those of experiments and discrete-based models (e.g., DEM) shows the accuracy of the presented model and its capabilities to deal with a broad range of granular flow regimes.

14th U.S. National Congress on Computational Mechanics
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Title: Stabilized Finite Element Method for Compressible Phase Change Phenomena

Author(s): *Ehsan Shams, Fan Yang, Yu Zhang, Chao Liu, Mark Shephard, Onkar Sahni, Assad Oberai, *Rensselaer Polytechnic Inst.*.

In many phase change phenomena that occur rapidly (cavitation, for example) the compressibility of the two phases plays an important role. The numerical simulation of these types of problems is challenged by the rapid motion of the interface, the enforcement of the appropriate flux conditions across the interface, and accounting for discontinuities in certain field variables. In this talk we present a finite element formulation that addresses these challenges. We weakly enforce the flux conditions at the interface, and account for discontinuities in field variables by using discontinuous interpolations that move with the interface. We explicitly track the interface, and update the mesh in the volume using a judicious combination of mesh motion (through the Arbitrary Lagrangian Eulerian approach) and mesh modification. We describe the overall methodology, and demonstrate its utility by solving some canonical phase change problems.

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Title: Elastic-Brittle-Plastic Analysis of Hoek-Brown Rock Using Mohr-Coulomb Failure Criterion

Author(s): *Shailendra Sharan, *Laurentian University*.

The Mohr-Coulomb (M-C) failure criterion, expressed in terms of the M-C parameters cohesion and the angle of internal friction of the material, is the most commonly used failure criterion in geotechnical engineering. This failure criterion has been implemented in most of the general purpose finite element software. However, this criterion may not be suitable for many types of rocks, particularly a jointed rock mass. For such rocks, the nonlinear generalized Hoek-Brown (GH-B) failure criterion [1] may be more appropriate. However, the nonlinearity of this failure criterion may result in an additional computational difficulty due to the non-convergence of solutions. Due to this and other reasons, to the author's knowledge, this failure criterion is not available in any general purpose finite element software. In order to circumvent these computational difficulties, recently, a novel method was proposed for the linearization of nonlinear failure criteria [2]. The method is based on an iterative procedure to compute the range of minor principal stress within the yielded zone. The range is initially assumed by using an elastic solution. The linearization is done by using the least-squares regression and the equivalent M-C parameters are determined. Then a more refined range of minor principal stress is determined by conducting the finite element analysis using the M-C failure criterion. The iterative procedure is continued until a convergence criterion is satisfied. The analysis was, however, restricted to elastic-perfectly plastic materials only. The objective of this paper is to extend the method for elastic-brittle-plastic rocks. The tangent method is used for the computation of the equivalent peak values of M-C parameters and the least-squares regression is used for the equivalent residual values. The effectiveness of the proposed method is demonstrated by analyzing stresses and displacements around underground openings for several cases using analytical solutions and a commercial finite element software. Both circular and non-circular openings and hydrostatic and non-hydrostatic in situ stresses are considered. The proposed iterative method is shown to be convergent and the results are found to be significantly more accurate than the existing methods. References: [1] Sharan, S.K., "Analytical solutions for stresses and displacements around a circular opening in a generalized Hoek-Brown rock", International Journal of Rock Mechanics and Mining Sciences, 45, 78-85, 2008. [2] Sharan, S.K., "An iterative method for the linearization of nonlinear failure criteria", Journal of Advances in Engineering Software, to be published, 2017.

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July 17-20, 2017, Montreal, Quebec, Canada

Title: Modeling of Interfacial Damage in FFT Solvers

Author(s): *Luv Sharma, *TU Eindhoven*; Ron Peerlings, Marc Geers, *TU Eindhoven*; Pratheek Shanthraj, Franz Roters, *Max-Planck Institute for Iron Research*.

We present a method to include interface specific mechanics in a FFT based crystal plasticity framework. The method is developed keeping in mind the application to multiphase polycrystalline materials. In order to capture the full three-dimensional state of stress inside the fracturing zone, an interphase band is introduced along the sharp interfaces. This band consists of the material points (also called the Fourier sampling points) in the vicinity of the interfaces. Within this band, the plastic constitutive behavior is inherited from the respective adjacent grains. In addition, to model the anisotropic kinematics associated with the cracking process, a damage eigen strain is introduced [1,2]. The eigen strain is constructed by appropriately mapping the crack opening strains (in tangential and normal modes) at the interfacial planes. The driving forces for these openings are the resolved tractions which act against a monotonously degraded resisting force (damage yield surface degradation). The degradation (damage) of the yield surface is modeled via a nonlocal damage variable [3] to avoid localisation of the damage within the band. The extent of nonlocality is chosen so that the damage is more or less uniform in the direction perpendicular to the band. We need to ensure that the model predictions are objective with respect to the band thickness. To this end, we demonstrate the scaling relations of the model parameters, first for a uniform opening case and then for a propagating crack. Finally, an application to a cluster of grains is shown. References: [1] O. Aslan, and S. Forest, 2009. Crack growth modelling in single crystals based on higher order continua. Computational Materials Science, 45(3), pp.756-761. [2] P. Shanthraj, B. Svendsen, L. Sharma, F. Roters and D. Raabe, 2017. Elasto-viscoplastic phase field modelling of anisotropic cleavage fracture. Journal of the Mechanics and Physics of Solids, 99, pp.19-34. [3] R. Peerlings, R. de Borst, W. Brekelmans, J. de Vree. Gradient enhanced damage for quasi-brittle materials. International Journal for Numerical Methods in Engineering 39, 3391–3403 (1996).

14th U.S. National Congress on Computational Mechanics
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Title: The Successive Node Snapping Scheme: A Method to Obtain Conforming Meshes for Propagating Cracks and Line Defects

Author(s): Yang Wan, Tianju Xue, *Yongxing Shen, *Shanghai Jiao Tong University*.

We introduce a novel method to construct conforming meshes for evolving curves in 2D and 3D with a given background mesh (a crack in a triangular mesh in 2D and a dislocation in a tetrahedral mesh in 3D). The core of the method is to project chosen nodes onto the evolving curve and to simultaneously relax the neighboring nodes, each time within the local area of a segment of the curve. Following the curve, we adjust each local area successively to obtain the mesh conforming to the entire curve. Thus we term the method the successive node snapping (SNS) scheme. The proposed method can handle the case of a simple rectifiable curve, either open or closed, and a complicated curve set with one or multiple junctions. In the procedure, only a portion of nodes of the background mesh are moved and the connectivity of the nodes remains unaltered. And the same background mesh can be utilized for a family of evolving curves with no a priori conformity requirements. Compared with another similar method called universal meshes [1][2][3], our method has a milder geometric requirement on the background mesh, such as allowing obtuse triangles. We provide examples with crack patterns in 2D and dislocation paths in 3D. [1] R. Rangarajan, A.J. Lew, Universal meshes a method for triangulating planar curved domains immersed in nonconforming meshes, Int. J. Numer. Methods Eng. 98 (4) (2014) 236–264. [2] R. Rangarajan, M.M. Chiaramonte, M.J. Hunsweck, Y. Shen, A.J. Lew, Simulating curvilinear crack propagation in two dimensions with universal meshes, Int. J. Numer. Methods Eng. 102 (3–4) (2015) 632–670. [3] Y. Shen, C. Wu, and Y. Wan. Universal meshes for a branched crack. Finite Elements in Analysis and Design 129 (2017) 53-62.

14th U.S. National Congress on Computational Mechanics
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Title: Distributed Mesh Infrastructure for Particle-in-Cell Simulations

Author(s): *Mark Shephard, Eisung Yoon, Kaushik Kalyanaraman, Seegyoung Seol, *Rensselaer Polytechnic Institute*.

Particle-in-cell (PIC) method are becoming more commonly applied to resolve fine scale physics in problems in which PDE based methods alone are not sufficient. In these simulation methods the motion of the particles is influenced by fields that are solved for on a mesh and the mesh fields are influenced by the field values associated with the particles in their current positions. Thus there is a strong coupling between the particle motion and mesh-based solution processes as the solution steps from an initial state to a final state. In many applications areas, in particular ones with complex geometries and highly varying and/or anisotropic fields, there is a desire to employ unstructured meshes for the field solutions. Since the operations on the particles, with typically number in the billions, dominate, both in terms of computation and total memory, the particles are always distributed. However, it is common to maintain a copy of the mesh, which currently may reach a million elements, and its fields, in each memory space across the parallel computer. However, the combination of more complex systems being analyzed, higher accuracy needed for the field solve, and finite memory per process, is driving a need to distribute the mesh. The focus of this presentation is to outline an approach being developed to support massively parallel PIC calculations on distributed meshes and to indicate the status of the implementation of the approach to support fusion plasma simulations. Key aspects of the approach being developed include: 1) A mesh distribution with sufficient overlaps to avoid inter-process communications during a particle push step; 2) Introduction of a mesh-to-particle infrastructure and algorithm control strategy; 3) Use of adjacency-based searches to replace spatially-based searches; 4) Coordinating gather/scatter operations and parallel mesh-based solve based on the distributed mesh. This distribute mesh infrastructure for PIC calculations is being implemented in the XGC fusion plasma code. A summary of this implementation and performance results will be presented.

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Title: Meshfree Modeling of Penetration of a Self-Consolidating High-Strength Concrete

Author(s): *Jesse Sherburn, William Heard, Sean Wade, Brett Williams, *U.S. Army ERDC*.

High-strength concrete (HSC) is of great interest to military researchers for various applications in protective structures. One of the key issues in the applicability of HSC in protective structure applications is ensuring the concrete is workable into complicated forms before curing. Recently, a self-consolidating high-strength concrete (SCHSC) was developed in order to produce an HSC with the workability of traditional self-consolidating concrete, but with the enhanced strength properties of an HSC [1]. In the same study, the SCHSC was characterized for quasi-static and dynamic stress states. Additionally, the SCHSC was subjected to penetration by spherical steel projectiles to quantify its ballistic resistance. This work will investigate modeling the penetration events of the SCHSC using the advanced fundamental concrete (AFC) model inside the reproducing kernel particle method (RKPM) code NMAP. The calibration of the AFC model to a suite of quasi-static and dynamic SCHSC experimental data will be presented. In addition, the micro-crack informed damage model (MIDM) of Ren et al. [2] will determine the tensile damage portion of the AFC model. This multiscale method uses a microcell calculation informed by x-ray microcomputed tomography scans to determine microcell stress and strain, which is then volume averaged using energy bridging to determine a macroscale damage evolution function. Simulations of the projectile penetration will be performed employing the calibrated AFC model inside NMAP, and the results compared to the experimental results. [1] Heard, W. F. 2014. Development and Multi-Scale Characterization of a Self-Consolidating High-Strength Concrete for Quasi-Static and Transient Loads. Ph.D. dissertation, Vanderbilt University, TN. [2] Ren, X., J.S. Chen, J. Li, T. R. Slawson, M. J. Roth. 2011. Micro-cracks informed damage models for brittle solids. International Journal of Solids and Structures 48: 1560-1571. * Permission to publish was granted by Director, Geotechnical and Structures Laboratory.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Novel Numerical Algorithm For Modeling Solidification Of Water

Author(s): *Hasan Shetabivash, Ali Dolatabadi, Marius Paraschivoiu, *Concordia University*.

Ice formation resulted from impact of supercooled water droplets poses serious safety issues for aircrafts. As a result, an accurate prediction of freezing process is of the utmost importance for the aerospace industry. In the current study a semi-implicit finite difference approach for solving heat equation in the presence of solidification is proposed. The model is based on expressing the latent heat source term as a modification of heat capacity. The common approach for dealing with the solidification is using an analytical function of enthalpy or a solid fraction as a function of temperature [1]. These approaches are valid only for solidification of alloys in which there exists a relatively wide mushy zone [2]. However, in the case of solidification of pure materials, there is a sharp jump at the interface which needs to be captured with the numerical simulations. In the present study, instead of using the analytical values, an approximation of the enthalpy derivation is proposed to deal with the sharp jump of the enthalpy at the interface. Available approximations alleviate some numerical oscillations, but for high resolutions, the discontinuity of the enthalpy still leads instabilities. Therefore, in order to achieve numerical stability a correction step is performed before updating the solid fraction field. The one dimensional Stefan problem is used for validation of the numerical approach. References [1] Bourdillon, A.C., Verdin, P.G. and Thompson, C.P., 2015. Numerical simulations of water freezing processes in cavities and cylindrical enclosures. Applied Thermal Engineering, 75, pp.839-855. [2] Voller, V.R. and Swaminathan, C.R., 1991. General source-based method for solidification phase change. Numerical Heat Transfer, Part B Fundamentals, 19(2), pp.175-189.

14th U.S. National Congress on Computational Mechanics
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Title: An Adaptive Sampling Method Based on Grassmann Manifold Variations

Author(s): Dimitris Giovanis, *Michael Shields, *Johns Hopkins University*.

Robust uncertainty quantification (UQ) in computational mechanics requires a simulation-based approach and a number of evaluations of the response that spans the range of all uncertainties involved. In most simulation methods, in order to identify the probability law of the solution, the number of repeated model evaluations needs to be large; making UQ of large-scale systems a computationally intensive task. This paper explores a new adaptive stochastic simulation-based method for UQ based on observing variations in the projection of the solution on the Grassmann manifold. In the proposed methodology, the singular value decomposition (SVD) of the high-dimensional solution at each sample point is evaluated with each set of basis vectors of dimension corresponding to a point on the Grassman manifold [1]. The input parameter space is then discretized into a set of simplex elements using a Delaunay triangulation as in the simplex stochastic collocation method [2]. Within each element, variations of the Grassman manifold are estimated by measuring the geodesic Grassman distances between the vertex subspaces. Elements with large variations on the Grassman manifold are subsampled and the elements refined. This is further compared with an approach in which the vertex subspaces are projected onto the tangent space where the distances are computed. The advantage of the latter is that the tangent space is flat and is therefore more amenable to interpolation [3]. [1] A. Edelman, T.A. Arias, S.T. Smith, The geometry of Algorithms with orthogonality constraints, SIAM J. Matrix Anal. Appl. Vol. 20, No 2, pp 303-353, 1998 [2] Witteveen, Jeroen AS, and Gianluca Iaccarino. "Simplex stochastic collocation with random sampling and extrapolation for nonhypercube probability spaces." SIAM Journal on Scientific Computing 34.2 (2012): A814-A838. [3] Amsallem, David, and Charbel Farhat. "Interpolation method for adapting reduced-order models and application to aeroelasticity." AIAA journal 46.7 (2008): 1803-1813.

14th U.S. National Congress on Computational Mechanics
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Title: Fatigue Crack Growth Simulation with Crack Closure Effect Using S-Version FEM

Author(s): *Yuto Shinozaki, Akiyuki Takahashi, *Tokyo University of Science*; Yuichi Shintaku, *University of Tsukuba*.

Owing to recent developments of computers and computer simulation techniques, fatigue crack growth simulation can be now performed using various computer simulation methods, such as finite element method (FEM), eXtended FEM (XFEM), s-version FEM (SFEM), even though the crack geometry and crack propagation path are complicated. However, because of a lack of understanding of the crack closure effect, the accuracy of the fatigue crack growth simulation, particularly of the growth rate, is still problematic, and remains an open issue to be solved. This paper presents two-dimensional fatigue crack closure simulations with crack closure effects using SFEM. Elastic-plastic analysis of cracked body is performed in order to obtain the crack opening level, and the resultant crack opening level is implemented into the Paris law. This process must be repeatedly done during fatigue crack growth simulation, and thus, to reduce the computational cost of the elastic-plastic analysis, the analysis is done only with local meshes, which are used in the SFEM for embedding cracks into the simulation volume. As validation of the proposed simulation system, the numerical results of elastic-plastic analysis only with the local mesh is compared with those obtained with a mesh for whole simulation volume. In addition, the crack tip element size is changed, and the numerical accuracy is examined. Finally, we demonstrate the fatigue crack growth simulation of a cracked specimen under a simple cyclic tension loading and discuss the crack closure effect on the crack growth rate.

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Title: Large Scale Coupled Analysis of Gas-Liquid-Solid Interaction Using ALE Mesh and Level Sets

Author(s): *Tatsuhiro Shono, Gaku Hashimoto, Hiroshi Okuda, *The University of Tokyo*.

Liquid-supported stretch blow molding (LSBM) is an advanced method to produce PET bottles. It has good mass-productivity because molding and filling processes are done simultaneously. Numerical simulation is indispensable because much trial and error are required to decide parameters for LSBM process. In LSBM process, fluid-structure interaction (FSI) is caused among injected liquid and a workpiece, and some bubbles also arise in the injected liquid. Zimmer et al. execute a FSI simulation using SPH and FEM for LSBM[1]. Large-scale parallel FSI simulation is required with a high resolution model because of the complex geometrical shapes of the workpiece (e.g. logo) and the bubble size. In this study, we propose a new coupling approach for FSI analysis[2] to predict extension of a workpiece in LSBM processes. The arbitrary Lagrangian-Eulerian (ALE) mesh is used to track the liquid-solid interface and the level set method is used to capture the gas-liquid interface on the ALE mesh. The level sets are reinitialized and the volume of liquid is corrected at each time step. The fields of structural displacement, fluid velocity and pressure are solved by a monolithic scheme. On the other hand, these fields and the level sets are solved by a partitioned scheme. The present method has been implemented into FrontISTR, which is an open source parallel FEM software for large-scale nonlinear structural analysis. A rotating oil tank problem[3] has been solved to verify the features of air-oil two-phase flow and large deformation of an elastic plate. In this problem, the rotation angle of an oil tank is vibrated with amplitude 4.0 degrees and period 1.21 seconds. The air-oil interface deformation and the tip displacement of the elastic plate are compared with experimental data and numerical results by other researchers. In this verification, applicability of the present method is shown to large-scale FSI problems. The rotating oil tank problem refined into more than millions nodes is solved for verification. [1] J. Zimmer, G. Chauvin, and M. Stommel: Experimental investigation and numerical simulation of liquid supported stretch blow molding, Polymer engineering and science, Vol. 55, No. 4, pp. 933-944, 2015. [2] T. Shono, G. Hashimoto and H. Okuda: Large-Deformation Fluid-Structure-Contact Interaction Analysis for Liquid Supported Blow Molding, FEF2017, Rome, Italy, April 5-7, 2017 (to be presented). [3] Botia-Vera E., Bulian, G. and Lobovsky, L. Three SPH novel benchmark test cases for free surface flows. In 5th ERCOFTAC SPHERIC Workshop on SPH Applications, 2010.

14th U.S. National Congress on Computational Mechanics
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Title: Use of the Fruchterman-Reingold Graph Embedding Algorithm to Untangle Hybrid Meshes

Author(s): Jake Quinn, Sanjukta Bhowmick, *University of Nebraska-Omaha*; *Suzanne Shontz, *University of Kansas*.

During finite element simulations, meshes can be deformed significantly, causing the mesh elements to become inverted or overlap with other elements. Meshes are said to be tangled whenever at least one of these events occur. Other causes of tangling include advancing front mesh generation, mesh smoothing or warping, and deformation of a low-order mesh to generate a high-order mesh. Mesh tangling is an issue in that it leads to non-accurate, non-stable solutions of partial differential equations via traditional finite element methods. Mesh untangling methods have been proposed to untangle finite element meshes. Most of the mesh untangling methods in the literature are based on geometry and/or optimization. Only a few approaches for mesh untangling using graph embedding are in existence. One such method is the force-directed graph embedding method of Shontz and Bhowmick [1] based on the Fruchterman-Reingold graph layout algorithm [2]. In [1], the Fruchterman-Reingold method in [2] is modified so that it can be used for mesh untangling. In particular, goals such as minimization of edge intersections and near equalization of edge lengths were introduced. These goals correspond roughly to mesh untangling and generation of good quality mesh elements. In our current work, we extend the method in [1] through two untangling paradigms. First, we untangle meshes constrained to a rectangular bounding box using a heuristic method of corner attraction to stabilize the mesh. Second, we untangle meshes with irregular but fixed boundaries in a sequential approach based on proximity to boundary vertices. We test the performance of our method on tangled finite element meshes including triangular meshes, quadrilateral meshes, and hybrid meshes containing both types of elements, in addition to 3D meshes. In our talk, we will present results which demonstrate the viability of our method when used to untangle finite element meshes with irregular boundaries, holes, and various element types. We will also present results pertaining to mesh quality. References: [1] S. Bhowmick and S.M. Shontz, “Towards high-quality, untangled meshes via a force-directed graph embedding approach”, Proc. of the 2010 International Conference on Computational Science, Procedia Computer Science, Volume 1, Issue 1, May 2010, p. 357-366. [2] T. Fruchterman and E. Reingold, “Graph drawing by force-directed placement”, Software Pract. Exper. 21 (1991) 1129-1164.

14th U.S. National Congress on Computational Mechanics
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Title: Stabilization of Peridynamic Correspondence Material Models

Author(s): *Stewart Silling, *Sandia National Laboratories*.

The peridynamic mechanical theory is a nonlocal generalization of classical continuum mechanics that applies to systems of discrete particles as well as continuous media with or without defects. Interactions between material points in a peridynamic medium are expressed in terms of bond force densities, which are determined by the deformation through a material model. The variety of material models available within the peridynamic theory include the correspondence materials. These use a stress tensor that is determined from a local material model with the help of an approximate deformation gradient tensor, which is evaluated from a nonlocal operator applied to the peridynamic medium. This approximate deformation gradient operator is non-invertible, meaning that many deformations of a neighborhood of a point can have the same approximate deformation gradient. This nonuniqueness creates practical difficulties in computations, manifesting itself in zero-energy mode instabilities, matrix rank deficiency, and vanishing wave speeds at certain finite wavelengths. Although many stabilization methods have been proposed, a new method has some desirable properties. It can be proven to eliminate the zero-energy mode instability in both a continuum model and its meshless discretization. The modification adds a term to the strain energy density in an elastic correspondence material model that penalizes departures of the deformation from a uniform deformation. Thus, all the deformations that have the same approximate deformation gradient tensor (as a result of the operator's non-invertibility) have higher energy than the one that exactly corresponds to a uniform deformation with this gradient. The new term, when mapped onto bond force densities through the Frechet derivative, has the remarkable property of leaving the net stress unchanged. The proposed new stabilization method is demonstrated to control zero-energy mode oscillations in numerical examples, generating more realistic fracture behavior in brittle materials. It also permits large deformations of ductile materials to be modeled with reduced oscillations. Dispersion relations show that the stabilized model eliminates the zero-velocity waves that are otherwise present in the correspondence models. The method applies to any correspondence material model and requires only modest changes to existing code.

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Title: Topology Optimization of an Axisymmetric Adsorbed Natural Gas Vessel with Phase Change Materials

Author(s): *Diego Silva Prado, *School of Engineering of the U*; Ricardo Cesare Romam Amigo, Emilio Nelli Silva, *School of Engineering of the University of São Paulo*.

Adsorption Technology is a promising alternative for gas transport and storage systems in which the gas is stored in the adsorbed form in a porous media know as "adsorbent". Although The drawback of Adsorption Natural Gas (ANG) systems is the reduced storage capacity when compared to other storage systems such as Compressed Natural Gas (CNG) and Liquefied Natural Gas. (LNG). Adsorption nature is exothermic, as the gas is adsorbed, heat is generated by the chemical reaction. As the temperature of the adsorbent increases, it becomes less attractive to the adsorption phenomena. Phase Change Materials (PCM) are advanced materials which can store significant amounts of energy during their phase change at a constant temperature. Studies show that when placed in the interior of an ANG vessel, PCM can improve the amount of stored gas and the amount of delivered gas. Additionally, these studies point that the amount and the geometry of PCM inside the vessels cause variation on the benefits brought by these materials. As a versatile tool for distributing material inside a domain, the topology optimization method is suitable for this employment. This work aims to perform the topology optimization of a slice of a cylindrical ANG vessel. The physical model consists of the heat, mass and internal energy equations of an ANG vessel with PCM in its interior. The boundary conditions are the natural convection on the vessel walls and the pressure and temperature input on the vessel extremity. The method employed to solve this problem is the finite element method (FEM) and the PDEs are handled by the FEniCS libraries. The sensitivities calculation is performed by dolfin-adjoint libraries. The Project variable is the amount of PCM mixture in each region of the vessel. The phase change phenomenon is modeled with the Finite Element Problem. The phase change enthalpy is modeled in the variational problem level. As there is a duality relationship between the amount of adsorbent to store gas and the amount of PCM to decrease the temperature, the topology optimization aims do find the best proportion between then. An experimental work from the literature is the reference for the model employed for this study. The results for the Axisymmetric model are presented and discussed.

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Title: GFEM Computations in Heterogeneous Solids Using Optimal Local Bases

Author(s): Robert Lipton, *Paul Sinz, *LSU*; Michael Stuebner, *UDRI*.

We apply optimal local bases functions identified in [1], [2] to computationally verify exponential convergence of the resulting Multiscale GFEM scheme. A battery of numerical examples are carried out for composite materials that demonstrate exponential convergence independent of contrast. The method is also applied to deliver a scheme for identifying worst case boundary loads that deliver maximum relative energy concentration around defects [3]. References [1] I. Babuska and R. Lipton, Optimal local approximation spaces for generalized finite element methods with application to multiscale problems, Multiscale Modeling and Simulation, SIAM, 9, 373-406, 2011. [2] I. Babuska, X. Huang, and R. Lipton, Machine computation using the exponentially convergent multiscale spectral generalized finite element method, ESIAM: Mathematical Modeling and Numerical Analysis, 48, 493-515, 2014. [3] R. Lipton, P. Sinz, and M. Sauebner, Uncertain loading and quantifying maximum energy concentration within composite structures, Journal of Computational Physics 325, 38–52, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: Continuous Integration for Large-Scale Scientific Software Development

Author(s): *Andrew Slaughter, *Idaho National Laboratory*.

The Multiphysics Object Oriented Simulation Environment (MOOSE) framework sits at the center of a large open source community while supporting very high software quality assurance standards. MOOSE's custom-built CI tool (CIVET) is essential for enabling concurrent development within its hierarchy of applications and the framework while ensuring individual application integrity and functional multi-project integration. This is accomplished through a multi-layer testing model that tests all combinations of development and stable branches of each application to pinpoint defects through simultaneous development efforts. CIVET's distributed client model and version controlled recipes enabled proper configuration management and scalable testing and reporting as the project continues to expand. This model allows mature application developers full control over their testing strategy without inhibiting contributions from less experienced developers. Our development model and custom integration tool will be demonstrated.

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Title: A Posteriori Error Estimation for Reduced Basis Approximation by the Method of Random Duals

Author(s): Anthony t. Patera, *M.I.T.*; *Kathrin Smetana, *University of Twente, M.I.T.*.

In this talk we present a probabilistic a posteriori error estimator for the reduced basis (RB) method for linear Partial Differential Equations (PDEs) that are inf-sup stable. The a posteriori error estimator presented does not require the estimation of the inf-sup or coercivity constant of the bilinear form of the considered PDE. One key ingredient of the a posteriori error estimator is the solution of a reduced dual problem with random right-hand side. Here, we extend the approach in [1], where the solution of an adjoint problem with random conditions at the final time is employed to estimate the approximation error for Ordinary Differential Equations. Both the a posteriori error estimator presented in this talk and the one introduced in [1] rely on the small sample statistical method as proposed in [2], which can in particular be used to estimate the norm of a vector by evaluating the inner product of this vector with certain random vectors. By employing the above we show that if the RB approximation error of the dual problem is small the error between the reference finite element solution and the RB primal approximation can be bounded, with high probability, from below and above by the a posteriori error estimator times a constant. Numerical experiments confirm the theoretical findings. References: [1] Y Cao and LR Petzold, A Posteriori Error Estimation and Global Error Control for Ordinary Differential Equations by the Adjoint Method, SIAM J Sci Comput, 26(2):359—374, 2004. [2] CS Kenney and J Laub, Small-Sample Statistical Condition Estimates for General Matrix Functions, SIAM J Sci Comput, 15(1):36—61, 1994.

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Title: The Impact of Myocardium Compressibility in Computational Simulations of the Healthy and Infarcted Heart

Author(s): *Joao S. Soares, David S. Li, Michael S. Sacks, *The University of Texas at Austin*; Eric Lai, Joseph H. Gorman III, Robert C. Gorman, *University of Pennsylvania*.

Myocardial infarction (MI) induces maladaptive remodeling of the left ventricle, causing dilation, wall thinning, change in mechanical properties, and loss of contractile function. In-silico based models of the heart allow to: (1) evaluate the effects of MI on cardiac function impairment; (2) understand etiology and pathophysiology of myocardium remodeling; and (3) improve virtual surgery, medical device development, and provide quantitative risk stratification tools. Material modeling of myocardium, and its critical numerical implementation, remains an area where much progress is required. One challenging feature is the interaction of coronary perfusion with myocardial contractility and compressibility. While volumetric changes in the myocardium during the cardiac cycle have been known to occur for at least two decades, their incorporation into cardiac simulations has yet to be fully accomplished. We have developed an in-silico model of MI based on extensive datasets from a single ovine heart. Magnetic resonance images (MRI) at end-diastole were segmented to create a finite element mesh. Diffusion tensor MRI (DTMRI) data was employed to prescribe principal fiber direction and to specify a transversely isotropic Fung-based hyperelastic model for the passive mechanical properties. The active stress responsible for myocardium contraction is time and space-dependent, and is driven by epicardial electrical activity experimentally measured with monophasic action potentials. The pressure-volume loop, measured through catheterization and sonomicrometry, was used to best-fit the modulation of active contraction. When myocardium is actively contracting during systole, progressive reductions of volume occur from the epi- to the endocardium and from the base to the apex. To account for these compressible effects, we have developed a specialized material model with a penalty term that allows for reductions in volume only and is modulated by the active contraction. The employment of a complete dataset from a single heart avoids unnecessary image registration between MRI and DTMRI images. The coupling between electrical activity and active contraction is significant to heart biomechanics and is needed to obtain physiological realistic heart function. The finding that perfused myocardium is compressible implies that results from analyses assuming incompressibility are not realistic. Not only incompressible ventricular walls are thicker at peak systole (as the relationship between fiber shortening and wall thickening is highly sensitive to volumetric changes), but also ventricular stresses will be substantially overestimated – the former is crucial for accurate representation of ventricular kinematics, whereas the latter is key to properly evaluate myofiber stress sparring, the most important biomechanical factor of ventricular remodeling.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Propagating Stochastic Manufacturing Processes into Risk Predictions for Gas-Turbine Engines

Author(s): *James Sobotka, Michael Enright, Kwai Chan, Craig McClung, John McFarland, Jonathan Moody, *Southwest Research Institute*.

This presentation proposes a tractable multiscale strategy to refine fracture risk predictions by propagating stochastic features of the manufacturing process into damage tolerance calculations for gas-turbine engine discs. The life of a gas-turbine engine disc may end by a rare but not improbable damage process: Cracks initiate from manufacturing and material anomalies, then grow by fatigue processes under cyclic loading, and finally fracture once the applied loading exceeds the toughness of the material. Due to the rarity of these anomalies that trigger this damage process, these discs are certified using a probabilistic approach that predicts the number of fractures in a large sample population. The damage process may be accelerated by microstructural features (i.e., grain size) or hindered by engineered residual stresses. These manufacturing effects (microstructure and residual stress) are in turn controlled by the non-deterministic manufacturing process parameters (e.g., cooling rate). Our strategy leverages computationally intensive software (i.e., DEFORM™) that uses manufacturing process parameters (e.g., cooling rate) as inputs to predict the microstructure and engineered residual stresses. Rather than simulate a new manufacturing process for every Monte Carlo simulation of a disc, our strategy develops a computationally efficient surrogate model of the manufacturing process that is calibrated from a limited number of deterministic analyses simulated prior to the fracture risk calculations. This strategy supports rapid predictions of the manufacturing effects that can then be propagated into the fracture risk during Monte Carlo sampling, i.e., by modifying residual stresses and by scaling fatigue crack growth processes based on the predicted microstructure. Consequently, the fracture risk predictions incorporate variability from the manufacturing process. Our strategy has been implemented within the probabilistic damage tolerance software DARWIN®. This presentation illustrates the first steps towards tailoring the manufacturing process to limit fracture risk. We demonstrate the impact of manufacturing processes on fracture risk local to a region and total fracture risk for the entire disc. In particular, we concentrate on the impact of engineered residual stresses (affects crack driving force), the average grain size (alters crack growth properties), and the as-large-as (ALA) grain size (affects crack formation properties). We discuss the scaling models that relate the predicted grain size to fatigue crack growth rates and formation rates. We also present our predictions of the microstructure, residual stress, and crack growth scaling over the disc. These results demonstrate potential benefits from integrated computational materials engineering (ICME) applied to the gas turbine engine design process.

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Title: Automated Simulation of the Multiscale Damage Response of Materials with Complex Microstructures

Author(s): *Soheil Soghrati, Anand Nagarajan, Fei Xiao, Bowen Liang, Hossein Ahmadian, Ming Yang, *The Ohio State University*.

We present a new non-iterative algorithm, named Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR), for creating high fidelity FE models of materials with intricate microstructure. CISAMR transforms a structured grid into a conforming mesh with appropriate element aspect ratios and negligible discretization error by combining customized versions of three algorithms: (i) Structured Adaptive Mesh Refinement; (ii) r-adaptivity of the nodes of elements intersecting with materials interfaces; and (iii) sub-tetrahedralization of the background elements affected by the previous two steps. While the complexity and computational burden associated with this process is comparable to those of creating integration sub-elements in mesh-independent methods such as eXtended/Generalized FEM (X/GFEM), CISAMR obviates the need for (and thus computational cost associated with) creating enrichment functions. Yet, similar to X/GFEM, CISAMR preserves the original structure of the background grid after the construction of the conforming elements, which highly facilitates modeling problems with evolving morphologies. Note that, unlike mesh generation algorithms such as Quadtree/Octree based techniques, CISAMR does not relocate any of the nodes of the background mesh other than those cut by the interface; thus no iterative smoothing or relaxation process would be necessary. We show that FE simulations relying on meshes generated using CISAMR yield the same levels of accuracy and convergence rates as those obtained using the Delaunay tessellation method. To enable the automation of the modeling process, CISAMR is integrated with a novel virtual microstructure quantification algorithm relying on a set of raw data extracted, for example, from micro-computed tomography images to build realistic virtual models of materials with heterostructures. The proposed technique implements a suit of algorithms including the Centroidal Voronoi Tessellation (CVT) and Genetic Algorithm (GA) to synthesize periodic microstructures with desired volume fraction, shape, size distribution and spatial arrangement of embedded heterogeneities. The Non-Uniform Rational B-Splines (NURBS) parametric functions are employed to characterize the intricate morphology of particles/fibers in the microstructure. In order to better utilize the inherent capability of NURBS, we also combine CISAMR with a generalized NURBS-enhanced mapping to eliminate the geometric discretization error in the resulting FE models. A unique feature of this new mapping is the ability to create geometrically exact conforming meshes without increasing the number of degrees of freedom. We demonstrate the application of the proposed modeling capabilities for simulating the multiscale damage response of several materials systems including carbon fiber reinforced polymer composites, heterogeneous structural adhesives, and ceramic fiber reinforced aluminum composites.

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Title: Effect of Geometry of Microfluidic on Hydrodynamic Single Cell Trapping

Author(s): *Ahmad Sohrabi Kashani, Muthukumaran Packirisamy, *Concordia University*.

Capturing and trapping of cells is the first critical step in single cell analysis to immobilize cells at a precise location for further analysis. At the same time, fluid flow needs to be applied to provide the cells with nutrients and other mediums influencing the behavior of the cells. Many microfluidic-based technologies have been developed to control the spatiotemporal of environmental of cells. Various forces such as magnetic, electrical, acoustic, optical and hydrodynamic could be implemented to manipulate the cells. Hydrodynamic trapping of cells offers low-cost, simple, efficient and high-throughput arraying of the cell without controlling or using equipment such as lasers, electrodes, magnets, and ultrasound transducers. In this technique, sample and medium are introduced through flow channels, so this method provides conditions to observe responses of the cells to the environmental changes. In this work, a hydrodynamic contact based lab on a chip is developed to immobilize single cells through positioning a series of micro-sieve on the sidewall of the main channel. In our design, micro-sieves and the concept of “path with the least resistance” are used to design main and side channels to enhance the probability of trapping. The design includes a main channel with inclined walls and two side channels. In contrast to other works, a channel with inclined walls is designed to increase the hydrodynamic resistance of the main channel as well as pressure differences between the main channel and side channels. As a result, microparticles have more propensity to pass through side trap sites comparing to the outlet of the main channel. Moreover, the main channel does not need to be extended long to generate higher flow resistance than trap sites. Not only the system can be more compact, but also residence time can be decreased. In this work, the computational fluid dynamic simulation analysis by COMSOL Multiphysics is used to optimize the geometrical parameters of channels and trap sites that impact the flow, and predict the fluid flow pattern inside the channels, considering the dimensions of target biological particles. Moreover, the trapping efficiency of trap sites within the microfluidic device is characterized using the numerical simulation. References: Valizadeh, A. and Khosroushahi, A.Y., 2015. Single-cell analysis based on lab on a chip fluidic system. Analytical Methods, 7(20), pp.8524-8533. Xu, Xiaoxiao, Zhenyu Li, and Arye Nehorai. "Finite element simulations of hydrodynamic trapping in microfluidic particle-trap array systems." Biomicrofluidics 7.5 (2013): 054108. Lawrenz, Anthony, Francesca Nason, and Justin J. Cooper-White. "Geometrical effects in microfluidic-based microarrays for rapid, efficient single-cell capture of mammalian stem cells and plant cells." Biomicrofluidics 6.2 (2012): 024112.

14th U.S. National Congress on Computational Mechanics
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Title: Geometrically Nonlinear Simulation of Carbon Nanotubes Using a Neural Network-Based Surrogate Modelling Technique

Author(s): *George Soimiris, *PhD candidate*; Vissarion Papadopoulos, *Associate Professor* ; Dimitrios Giovanis, *Dr* .

This study presents a geometrically nonlinear surrogate modelling technique based on neural networks, which is able to simulate the behavior of carbon nanotubes (CNTs) by using a series of equivalent beam elements (EBE). CNTs with small length to diameter ratios exhibit cross sectional distortions that cannot be captured even by advanced beam theories. To this purpose, a CNT structure simulated according to the molecular structural mechanics (MSM) approach is replaced by a series of NN-based nonlinear EBEs that are capable to capture the aforementioned higher-order phenomena. A portion of the total length CNT is subjected to a large number of geometrically nonlinear analyses having as inputs displacement vectors in the range of minimum and maximum end section displacements occurring at a supportive model consisted of a series of classical nonlinear beam elements instead, while the outputs are the corresponding reaction forces. These displacement vectors are then used as inputs, while the reaction forces vectors as outputs, in the neural network training procedure. According to the above, the NN surrogate model is properly trained to return accurate enough estimates of the EBE internal forces in the range of the applied CNT portion end deformations. By describing the problem in the framework of a standard geometrically nonlinear co-rotational beam formulation within a Newton-Raphson incremental-iterative scheme, the residual is accurately and efficiently provided by the NN approximation of the computationally expensive MSM model. Following this technique it is possible to predict the nonlinear response of complex system in a fraction computing time.

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Title: Manifold Sampling for Data-Driven UQ and Optimization

Author(s): Roger Ghanem, *USC*; *Christian Soize, *U Paris-Est*.

We describe a new methodology for constructing probability measures from observations in high-dimensional space. A typical challenge with standard procedures for similar problems is the growth of the required number of samples with the dimension of the ambient space. The new methodology first delineates a manifold in a space spanned by available samples, then it constructs a probability distribution on that manifold together with a projected Ito equation for sampling from that distribution. A demonstration of this new methodology to problems in uncertainty quantification, and in design optimization under uncertainty will be shown.

14th U.S. National Congress on Computational Mechanics
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Title: Techniques for Linking One-Way Coupled and Fully Coupled Simulations of Flow-Induced Vibration

Author(s): *Jerome Solberg, Kei Mueller, *Lawrence Livermore Nat'nl Lab*.

Flow-induced vibration is a significant engineering challenge, especially in the design of heat exchangers. The desire for increased efficiency and decreased plant footprint and cost necessitate thinner walled tubes, longer spans, greater packing density, and higher flow velocities. All these features lead to greater fluid-structure interaction, with the concomitant need for improved analytical tools. One approach common within the industry is one-way-coupled analysis, where the flow pressure loads, varying in time, are applied to the structure. The response of the fluid to structural motions is approximated via “added mass” and “added damping” terms included in the structural equations. These terms are generally a function of the fluid and the geometry, and can be difficult to calculate even for simple geometries [1]. Forward coupled analyses have great utility within the design cycle, but at high enough velocities a fully-coupled approach is necessary. A staggered approach is desirable because they allow disparate fluid and structural solvers to be coupled together while treating each solver as a “black box” in relation to the other. Such schemes can be slow to converge (or even not converge at all), because at low stiffness values of the structural components correct accounting for the “added mass” term is critical, as the well-known analysis of Causin and his coworkers has demonstrated. Recently, a related concept, that of “fictitious mass/damping” has been used in the context of a fully-coupled analysis where the fluid and structure solvers are solved in a staggered scheme incorporating relaxation [2]. In this work, we examine approaches based initially on [2] where the added mass/damping terms are monitored based on the progress of the solution. Solution strategies based on Quasi-Newton methods [3] are also explored, and the results from both approaches used to calibrate one-way-coupled analyses. The advantages of each of these methodologies are compared, with a special focus on their ability to inform one-way-coupled analyses. References: [1] Wambsganss, M. W., Chen, S.S., and Jendrzejcyk, J.A., 1974, "Added mass and damping of a vibrating rod in confined viscous fluid" ANL-CT-75-08, Report, Argonne National Laboratory, Argonne, Illinois. [2] Baek, H. and Karniadakis, G. E., “A convergence study of a new partitioned fluid-structure interaction algorithm based on fictitious mass and damping,” Journal of Computational Physics, 231 (2012), 629-652. [3] Bogaers, A. E. J., Kok, S., Reddy, B. D. and Franz, T. “Quasi-Newton methods for implicit black-box FSI coupling” Comp. Meth. in Appl. Mech. and Eng., 279 (2014), 113-132.

14th U.S. National Congress on Computational Mechanics
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Title: From Digital Images, STL and NURBS to Computational Stress Analysis Using Scaled Boundary Polytope Elements

Author(s): *Chongmin Song Song, *UNSW Sydney, Australia*.

The process of computational stress analysis includes the discretization of the geometric models and the solution of partial differential equations reformulated as a system of algebraic equations for the discretized systems. In the popular finite element method, a geometric model is discretized into a mesh of elements of simple geometries (triangles and quadrilaterals in 2D, and tetrahedrons and hexahedrons in 3D). With increasingly affordable computer power, the human effort required in the mesh generation becomes more and more critical in terms of both cost and time, especially when moving boundaries are involved. At the meantime, the digital images and STL format are increasing popular in computer simulation owing to the rapid advances in digital imaging technologies and 3D printing. Most traditional techniques for mesh generation of CAD models are not directly applicable. This presentation covers the development of the scaled boundary polytope elements and their application aiming to fully automate the process of computational stress analysis starting from geometric models. The general polytope (polygon in 2D and polyhedron in 3D) elements can have any number of faces, edges and vertices and offer a much higher degree of flexibility in mesh generation than standard finite elements. This allows the development of a polytope mesh generator based on the simple and efficient quatree/octree algorithm. Geometrical models given as digital images [1], STL models [2] and traditional CAD models [3] can be handled in a unified approach. The whole analysis process is fully automatic. The efficiency, robustness and some salient features of the proposed technique will be demonstrated. Potential research and applications of this novel technique will be discussed. References: 1. Saputra, A., Talebi, H., Tran, D., Birk, C. and Song, Ch. (2017) “Automatic image-based stress analysis by the scaled boundary finite element method”, International Journal for Numerical Methods in Engineering, 109:697–738. 2. Liu, Y., Saputra, A. and Song, Ch. (2017) “Automatic polyhedral mesh generation and scaled boundary finite element analysis of STL models”, Computer Methods in Applied Mechanics and Engineering, 313:106–132. 3. Talebi, H., Saputra, A. and Song, Ch. (2016) “Stress analysis of 3D complex geometries using the scaled boundary polyhedral finite elements”, Computational Mechanics, 58:697–715.

14th U.S. National Congress on Computational Mechanics
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Title: Atomistic Investigation and Continuum Model Prediction of Hydrogen Diffusion along Grain Boundaries

Author(s): Xiao Zhou, *Jun Song, *McGill University*.

Hydrogen embrittlement (HE) has been a long-standing challenge for the high-strength structural metals. One key aspect in HE is the kinetics of hydrogen at microstructures, e.g., grain boundaries (GBs), which is vital to accurate prediction of HE threshold and material deformation/fracture behaviors. However, Kinetics of hydrogen at grain boundaries (GBs) remains an open question and conflict opinions exist despite great amount of research works. In this study, we employ first-principles density functional theory calculations in combination of novel space tessellation techniques and Kinetic Monte Carlo to systematically investigate the complex interaction between hydrogen and GBs regarding energetics and kinetics. Our findings indicate that the migration barriers and connectivity of hydrogen at GBs are strongly dependent on local GB structures. In particular, hydrogen can exhibit two distinct types of kinetics, evidencing the dual role of GBs in hydrogen kinetics. A simple model based on the Frank-Bilby dislocation description of GBs is proposed to mechanistically clarify such behaviors of hydrogen kinetics at GBs, and identify the key structural characteristics prescribing hydrogen diffusivity along GBs. Our results can provide critical new clues and a multiscale framework towards quantitative understanding of hydrogen kinetics at microstructures.

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Title: Application of the Particle Difference Method (PDM) for Predicting Solidification of Polycrystalline via Diffusive Interface Approach

Author(s): *Jeong-Hoon Song, Ashkan Almasi, *University of Colorado Boulder*; Tae-Yeon Kim, *Khalifa University, UAE*; Young-Cheol Yoon, *Myongji College, South Korea*.

This study presents an application of the particle difference method (PDM) [1-3] to the simulation of the solidification process of polycrystalline based on the diffusive interface approach such as the multi-phase field model (MPFM). In order to evaluate the computational feasibility of the strong form-based meshfree particles method to the MPFM, the PDM is applied to the simulation of the polycrystalline growth initiating from the undercooled melt materials. The coupled partial differential governing equations that describe the growth of the material grains with different orientations and the evolution of the temperature field with the latent heat are directly discretized with the PDM approach in terms of the numerically computed differential operators. The PDM is able to directly discretize the strong form of the governing equation without aids from the weak form, and construct globally continuous interpolated and its derivative fields. As one of distinct features of the method, the PDM obtains higher-order derivatives of the shape functions in the process of the calculation of shape functions without excessive extra cost, unlike other conventional meshfree and collocation methods. With the benchmark problem in the solidification of pure Ni material system, we present a detailed description of the PDM as well as its numerical accuracy and convergence at various discretization levels. References: [1] Y.C. Yoon and J.H. Song, “Extended particle difference method for moving boundary problems”, Computational Mechanics, 54:723–743 (2014). [2] Y.C. Yoon and J.H. Song, “Extended particle difference method for weak and strong discontinuity problems: Part II. Formulations and applications for various interfacial singularity problems”, Computational Mechanics, 53:1105-1128 (2014). [3] Y.C. Yoon and J.H. Song, “Extended particle difference method for weak and strong discontinuity problems: Part I. Derivation of the extended particle derivative approximation for the representation of weak and strong discontinuities”, Computational Mechanics, 53:1087-1103 (2014). [4] Y. Fu, J.G. Michopoulos and J.H. Song, "Bridging the multi-phase field model with the molecular dynamics for the solidification of nano-crystals", Journal of Computational Science, http://dx.doi.org/10.1016/j.jocs.2016.10.014.

14th U.S. National Congress on Computational Mechanics
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Title: The Shifted Boundary Method: A New Approach to Embedded Domain Computations

Author(s): *Ting Song, Alex Main, Guglielmo Scovazzi, *Duke University*.

We present a new embedded boundary method for wave equation problems in time domain. Embedded boundary methods obviate the need for continual re-meshing in many applications involving rapid prototyping and design. Unfortunately, many finite element embedded boundary methods for incompressible flow are also difficult to implement due to the need to perform complex cell cutting operations at boundaries, and the consequences that these operations may have on the overall conditioning of the ensuing algebraic problems. We present a new, stable, and simple embedded boundary method, which we call “shifted boundary method” (SBM), that eliminates the need to perform cell cutting. Boundary conditions are imposed on a surrogate discrete boundary, lying on the interior of the true boundary interface. We then construct appropriate field extension operators, with the purpose of preserving accuracy when imposing the boundary conditions. We demonstrate the performance of the proposed method in simulations of problems in acoustics and shallow water flows.

14th U.S. National Congress on Computational Mechanics
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Title: Coupled CFD/CSD Simulations of Dust Production by Fragmenting Charges Using Stabilized Linear Tetrahedral Elements

Author(s): *Orlando Soto, Joseph Baum, *Applied Simulations Inc.*; Rainald Lohner, *George Mason University*; Robert Frank, *Applied Research Associates, Inc.*.

This paper presents the results of coupled Computational Fluid Dynamics (CFD)/Coupled Structural Dynamics (CSD) simulations of internal detonations of cased munitions against reinforced concrete walls. These simulations are part of a test, analysis, and modeling effort studying air blast propagation through breached walls. The coupled CFD/CSD simulations are providing additional insight and details not measured in the tests, as well as developing a synthetic database to supplement the test matrix. The simulations are performed to calibrate the CFD/CSD model and to determine the physic impacting the internal environments, wall breach, and blast propagation through the breach. Here we modeled the response of two reinforced concrete walls to loads from a cased charge, placed in close proximity to the center of wall 1. In the test, the detonation room (composed of two culverts) incurred a large amount of plastic damage due to the fragments and blast load, and both culverts failed. Test wall 1 initially breached over the middle third, with the wing walls removed by the later time blast loads. Debris from test wall 1 impacted test wall 2, which failed under the combined blast and debris. Initial coupled CFD/CSD simulations modeled the culverts as rigid, non-responding surfaces. These simulations reproduced the damage to the test walls, but the pressure histories matched the experimental data only out to 10 ms. Subsequent airblast reflections were significantly reduced, as if a large amount of energy has been evacuated from the facility. Post-test damage analysis showed significant fragment damage to the culverts, with the concrete stripped to the first layer of rebars. We estimate that the fragment impacts produced several hundred kilograms of dust that was ejected into the room. Repeat simulations, where the culvert response was modeled and the dust was allowed to absorb both kinetic and thermal energy, matched the experimental data significantly better. Initially, the simulations were performed with standard Finite Element methods (hourglass stabilized Belytschko-Flanagan hexahedral elements). However, the relatively recent developments of stabilized linear tetrahedral elements for non-linear CSD applications (See [1] and references therein) have shown a great improvement on capturing plastic localization zones and, therefore, fracture prediction in benchmarks problems. Hence, this work addresses how the implementation of such techniques improves the accuracy and the computer time savings for real life applications. Finally, comparisons with experimental data are presented to validate the numerical schemes (See [2] for details of the CSD/CFD coupling and fracture/fragmentation schemes). REFERENCES [1] Cervera, M., Chiumenti, M., Benedetti, L., Codina, R. "Mixed stabilized finite element methods in nonlinear solid mechanics. Part III: Compressible and incompressible plasticity". Computer Methods in Applied Mechanics and Engineering, 285, 752-775 (2015). [2] Soto, O.A., Baum, J.D., Löhner, R. ”An efficient fluid-solid coupled finite element scheme for weapon fragmentation simulations”. Eng. Fracture Mech., 77, 549-564 (2010).

14th U.S. National Congress on Computational Mechanics
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Title: Stabilized XFEM and FEM for Free Surface Incompressible Flows

Author(s): *Azzeddine Soulaïmani, Mamadou Touré, Adil Fahsi, *École de technologie supérieur*.

Free surface flows are examples of moving interface flow problems commonly encountered in nature and industry. Numerical methods capable of simulating such problems are usually classified as Lagrangian or Eulerian methods. In the Lagrangian approach, the mesh is partially or totally mobile. Eulerian methods include the Front-tracking and the Front-capturing methods. The Front-capturing methods, such as the Volume of fluid method (VOF) or the Level set method with their variants, are based on the evolution of a scalar function that is related to the interface position. The principle numerical difficulties are due to the jumps in fluid density and viscosity across the interface. A straightforward use of the finite element method to solve such problems leads to poor results since spurious currents are induced close to the interface. A simple remedy very often used is the smoothing the fluid properties inside the intersected elements by the interface. This approach is appealing since a legacy finite element solver for a single phase can be easily extended to two phase and free surface flows. However the spurious currents still appear although with a smaller magnitude. The eXtended Finite Element Method (XFEM) initially developed for crack problems by addresses these difficulties by enriching the approximation space to represent a known type of discontinuity in element interiors. The main drawback of XFEM is the ill-conditioning of the resulting system, and the tedious implementation effort required to ‘enrich’ a legacy Navier-Stokes solver, especially for 3D. In this work, the standard finite element method and XFEM are stabilized by additional force terms around the interface and by using a proper integration scheme for the cut elements. Several numerical tests for free surface flows are used to compare the results of both methods. REFERENCES T. Belytschko and T. Black (1999): « Elastic crack growth in finite elements with minimal remeshing ». International Journal for Numerical Methods in Engineering, 45 601-620. M. Touré and A. Soulaïmani (2016) « Stabilized finite element methods for solving the level set equation without renitialization ». Computers & Mathematics with Application, Volume 71, issue 8, pp 1602-1623.. M. Touré and A. Soulaïmani (2016) « Stabilized finite element methods for solving the level set equation with mass conservation». International Journal of Computational Fluid Dynamics ,Volume 30, issue 1, pp 38-55.

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Title: Penetration Modeling of Ultra-High Performance Concrete Using a Multiscale Meshfree Method

Author(s): *Paul Sparks, Jesse Sherburn, William Heard, Brett Williams, Patrick Kieffer, *U.S. Army ERDC*.

Terminal ballistic performance of concrete is of extreme importance to the military and civil communities. Over the past few decades, ultra-high performance concrete (UHPC) has been developed for various applications in the design of protective structures, since UHPC has an enhanced ballistic resistance over conventional strength concrete. Developing predictive numerical models of UHPC subjected to penetration is critical in understanding the material's enhanced performance. The current study presents a novel numerical investigation that compares recent experimental testing to computational simulations. This study employs the advanced fundamental concrete (AFC) model [1], and it will run inside the reproducing kernel particle method-based code known as Nonlinear Meshfree Analysis Program (NMAP). NMAP is advantageous for modeling impact and penetration problems that exhibit extreme deformation and material fragmentation. A multiscale meshfree method, which incorporates homogenization of the microstructure, is used to model UHPC. To improve the accuracy of the model, the microstructure calculations include statistical distributions derived from X-ray micro-computed tomography scans of cored UHPC samples. The evolution of failure in the microstructural calculations utilizes experimentally motivated data to drive the microcrack-informed damage model [2]. From the microstructural calculations, a damage evolution law is derived based on energy bridging between the cracked microstructure and the homogenized continuum. This damage evolution law and the calibrated AFC model will be used to numerically investigate ballistic panel penetration testing. Results of the numerical simulations will be compared to analogous experimental data. [1] Adley, M.D., A.O. Frank, K.T. Danielson, S.S. Akers, and J.L. O'Daniel. 2010. The Advanced Fundamental Concrete (AFC) model. Technical Report ERDC/GSL TR-10-51. Vicksburg, MS: U.S. Army Engineer Research and Development Center. [2] Ren, X., J.S. Chen, J. Li, T.R. Slawson, and M.J. Roth. 2011. Micro-cracks informed damage models for brittle solids. International Journal of Solids and Structures; 48: 1560-71. * Permission to publish was granted by Director, Geotechnical and Structures Laboratory.

14th U.S. National Congress on Computational Mechanics
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Title: Converting Faceted Data to B-Reps

Author(s): *Paul Stallings, *Sandia National Laboratories*.

An algorithm is presented that will convert two dimensional simplicial complexes to B-Reps. Input may include both manifold and non-manifold complexes that optionally may enclose a volume. Analytic surfaces are identified and created along with NURB surfaces for the non-analytic parts. Considerable effort is taken to make light weight surfaces, while also maintaining connectivity and tangency where appropriate. In addition, the non-analytic surfaces are smoothed with a tolerance that is based on the size of the given triangles. This algorithm finds larger, more human intuitive, faces instead of the smaller more random faces that some other algorithms find, which potentially allows the created faces to be grouped into editable features. Most of the algorithm can be run in parallel, and a significant amount of work has been done to optimize its performance on large models. The algorithm consists of first separating the analytic and organic parts from each other, and then cutting the organic parts up so that relatively simple surface covering techniques can be used to cover the parts while maintaining the needed continuity. The output of this algorithm is a STEP file or a part in any geometric modeler that supports B-Reps.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Mapping Error Quantification and Adaptive Remeshing for Large-Deformation Solid Mechanics

Author(s): *Andrew Stershic, *Sandia National Laboratories*.

For many problems in large-deformation mechanics, remeshing presents an attractive solution for addressing the issue of high mesh distortion. This approach necessitates a consistent mapping of state variables and internal state variables from the distorted source mesh to the new target mesh. Integration point quantities on the source mesh are extended to the entire domain through an L2 projection and interpolated to the target discretization. We discuss an approach implemented to quantify this mapping projection error and then adaptively refine the mesh accordingly to reduce error propagation. This process is applied to several large-deformation simulations with remeshing in SIERRA, a scalable multiphysics finite element code, to demonstrate its effectiveness in reducing the mapping error. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Implementing Generalized Adjoint Capabilities in libMesh

Author(s): Vikram Garg, *Roy Stogner, *The University of Texas at Austin*.

The Finite Element library libMesh supports generalized adjoint capability for both error-estimation and sensitivity calculation. Key challenges encountered in the addition of these capabilities included handling adjoint Dirichlet boundary conditions, which are critical for the computation of appropriate adjoints for boundary flux QoIs, and handling stabilized variational formulations, where the appropriate residual and enriched FE space have to be used to obtain accurate error estimates. We discuss how these challenges were overcome and the implementation of their solutions in libMesh.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: An Iterative Method for Multiscale Composite Structures

Author(s): Robert Lipton, Paul Sinz, *Louisiana State University*; *Michael Stuebner, *University of Dayton Research Institute*.

In this presentation we describe a new iterative method using optimal local approximation spaces for the extraction of stress and strain in multiscale heterogeneous materials. These local approximation spaces were developed in recent work of Babuska and Lipton [2] for the multiscale spectral generalized finite element method (MS-GFEM). The approximation spaces must be computed for each geometry and set of material properties being considered and are computationally expensive. The iterative method described here aims to reduce the number of local shape functions that need to be computed while maintaining a desired accuracy level. The method is presented in the framework of domain decomposition methods and employs overlapping domains within the Partition of Unity Method [1],[3]. Theoretical near-exponential convergence rates are provided for the iterative method and computational results are discussed and compared with experimental data. [1] I. Babuska, G. Caloz, and J. E. Osborn, Special finite element methods for a class of second order elliptic problems with rough coefficients, SIAM J. Numer. Anal. 31 (1994), pp. 945–981. [2] I. Babuska and R. Lipton, Optimal local approximation spaces for generalized finite element methods with application to multiscale problems, Multiscale Modeling and Simulation, SIAM, 9, 373-406, 2011. [3] I. Babuska and J. Melenk, The partition of unity finite element method, Internat. J. Numer. Methods Engrg., 40 (1997), pp. 727–758.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Asynchronous Space and Time Algorithm for Localized Uncertainty Quantification

Author(s): *Waad Subber, Karel Matous, *University of Notre Dame*.

For engineering problems with localized phenomenon, the computational cost of uncertainty quantification (UQ) can be reduced by confining the random variability of the model parameters within a region of interest. In the region of interest, a stochastic model with high resolution mesh and time discretizations is used. In contrast, apart from the region of interest, low spatial and temporal discretizations are allowed for a lower resolution stochastic model. To this end, we propose a customized intrusive polynomial chaos based solver with the capability of asynchronous treatment of the stochastic, spatial and temporal resolutions. In particular, we allow each subregion to have its local uncertainty representation and the corresponding mesh and time resolutions. Therefor, computing power can be directed toward a region of interest, where a stochastic model with high spatial and temporal resolutions is required. We verify our algorithm and study different scenarios to reduce the computational cost of UQ. For the linear elastodynamics problem, the algorithm shows a second order convergence rate in space and time for both the mean and the standard deviation of the displacement as well as the velocity. A projectile impacting a composite sandwich plate is considered as an engineering application for the proposed method.

14th U.S. National Congress on Computational Mechanics
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Title: Accuracy in Meshfree GFDM Schemes for the Incompressible Navier-Stokes Equations

Author(s): *Pratik Suchde, Joerg Kuhnert, *Fraunhofer ITWM*; Sudarshan Tiwari, *University of Kaiserslautern*.

In this talk, we consider sources of inaccuracy in meshfree Generalized Finite Difference Method (GFDM) schemes for fluid flow simulations. Specifically, we consider the problems of inconsistency in the div-grad operator (specific to strong-form meshfree methods) and inaccuracy at and near boundaries. We present methods to improve local accuracy in these regards. This corresponds to improved accuracy for both the velocity and the pressure field, without resorting to higher order methods. To improve accuracy in the velocity approximations, we show that solving an over-determined system (in a least squares sense) enables us to solve for the conservation of mass directly, rather than only indirectly via a pressure-Poisson system. This decouples the errors in the div-grad system from the mass conservation condition. Further, in the final pressure step, accuracy is improved by avoiding the pressure-Poisson equation by solving the momentum equation directly for the pressure gradient.

14th U.S. National Congress on Computational Mechanics
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Title: Dislocation Dynamics Modeling of Fracture Toughness and Plasticity at Crack Tip

Author(s): *Hayato Sugasawa, Akiyuki Takahashi, *Tokyo University of Science*.

Embrittlement of metallic materials is a critical issue for ensuring the safety and reliability of structures. The fundamental mechanism of embrittlement and ductile-brittle transition of metallic materials is believed to be relevant to the dislocation behavior, particularly in the immediate vicinity of crack tip. The fracture toughness might be controlled by the dislocation shielding effect given by the dislocations nucleated from the crack tip. Thus, for understanding the plasticity at the crack tip, and evaluating accurately the fracture toughness of materials, the behavior and elastic field of dislocations must be carefully taken into account. This paper presents the dislocation dynamics (DD) modeling of fracture toughness and plasticity of metallic materials at the crack tip. Cracks are modeled with a collection of dislocations, and the plasticity at the crack tip is simulated using the DD method. The dislocation shielding effect can be automatically accounted for in the simulations as the elastic interaction between the dislocations providing the plasticity and those describing the cracks. Using the DD model, fracture toughness change at low temperatures is simulated.

14th U.S. National Congress on Computational Mechanics
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Title: A Class of Examination of Simulation for Ductile Fracture

Author(s): *Hirofumi Sugiyama, Kazumi Matsui, Takahiro Yamada, *Yokohama National University*.

In this study, we examine the simulation method for ductile fracture, which enables to simulate from the occurrence of strong discontinuity to the final state of material. Estimating the evolution of failure in material and structure is the basic interest in many fields of the engineering. Recently, the finite element simulations play important roles to predict the mechanical behavior of structures, and material models have devised to approximate the phenomena. However, the ductile fracture is one of the unsolved problem in the fracture mechanics. The continuum damage mechanics have been developed for predicting the macroscopic material behavior. For example, Gurson-Tvergaard-Needleman(GTN) model and Lemaitre damage models are commonly accepted in our engineering fields to simulate the ductile behavior of metals. These models assume that the microscopic voids govern the ductile fracture and that their mechanisms consists of a few major steps. The so-called damage parameters are major state variables, hence their evolution laws are main interests in these kinds of mathematical models. However, these models cannot describe the discontinuities (cracks) clear because the damage variables merely treat as the variable and the discontinuities seem to be immersed boundary. On the other hand, we focus on the numerical simulation methods. The conventional finite element simulation is not good at handling the discontinuous field, because the finite element simulations describes the discontinuities by element boundaries. Therefore, generalized finite element method have been developed in computational fracture mechanics. Extended finite element method(X-FEM) is well-known method to simulate the crack propagation mainly in the linear elastic bodies. This method can easily simulate the nucleation and growth of discontinuities (cracks) by the character of enhanced approximation function. Thus, the X-FEM is hard to describe the discontinuities. By contrast, finite cover method (FCM) is one of the candidates to describe the discontinuities. The FCM defines multiple covers, which based on the concept of this method. To simulate the ductile fracture, we implement the simplified Lemaitre damage model to our FCM codes. The comparison of the load vs. displacement curve between conventional Lemaitre model and proposed one show the major difference after discontinuities occurs. More specifically, the proposed simulation shows that the load value dramatically reduced after occurrence of discontinuities, whereas the conventional one shows the gradually reduced. It is because the proposed method treats the load with multiple covers. Then some numerical examples show the capabilities the method in typical ductile failure of metal materials.

14th U.S. National Congress on Computational Mechanics
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Title: Modeling Strong and Weak Discontinuities without Element-Partitioning in the Extended Finite Element Method

Author(s): Eric B. Chin, *N. Sukumar, *UC Davis*.

In this talk, we model strong discontinuities (cracks) and weak discontinuities (holes and material interfaces) in two-dimensional linear elastic continua using the extended finite element method without the need to partition the enriched elements that are cut by the interface. For crack modeling, the standard finite element approximation is enriched with a discontinuous function and the near-tip crack functions. Rectilinear and curved interfaces are represented as level set functions whose nodal values are used to construct a finite element representation (piecewise algebraic curve) of the interface. To model a material interface in an elastic continua, the standard finite element displacement approximation is enriched through the framework of partition-of-unity with a function whose normal derivative is discontinuous across the interface. An element that is cut by the interface is decomposed into two polygons, which in general have affine and curved sides. We use Euler's homogeneous function theorem and Stokes's theorem to numerically integrate homogeneous polynomials on convex and nonconvex regions [1]. For contributions to the stiffness matrix, exact contributions are computed on simple polygons, and for polygons with curved sides, we only require a one-dimensional quadrature rule along the curved side. Hence, neither tree-based techniques for interface reconstruction nor element-partitioning on either side of the interface are needed. Unstructured linear triangular meshes and structured meshes consisting of rectangular finite elements are used. We demonstrate the accuracy and efficiency of the integration scheme and showcase several numerical examples with cracks, holes, and bi-material interfaces. References: [1] Chin E.B., Lasserre J.B., Sukumar N. “Numerical integration of homogeneous functions on convex and nonconvex polygons and polyhedra,” Computational Mechanics, vol. 56, pp. 967—981, 2015.

14th U.S. National Congress on Computational Mechanics
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Title: Hybrid Data-Driven Multiscale Computational Geomechanics across Length Scales

Author(s): *Waiching Sun, Kun Wang, *Columbia University*.

We present a hybrid data-driven approach to model multi-physical processes in fluid-infiltrating porous media across length scales. Unlike single-physics problems where a data-driven model is often used as a replacement of the solid constitutive law, a hydro-mechanical problem often leads to more complex hierarchical relations among physical quantities which in turn complicate the design of the data-driven solver. When artificial neural network is used, additional issues may arise when constraints and rules, such as material frame indifference, cannot be explicitly enforced without artificially expanding the training dataset. In this work, we introduce a component-based strategy in which a multiphysical problem is viewed as a directed graph, a network consisting of interconnected vertices representing physical quantities. This strategy enables modelers to couple data-driven model with conventional mathematical expression methods by considering different hierarchical relations among data. Depending on the availability of data, hybridization of data-driven and mathematical models may take different forms. To enforce material frame indifference efficiently, we employ spectral decomposition to handle the invariant and spin terms via Lie algebra.

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Title: A Mixed FEM for the Quad-Curl Eigenvalue Problem

Author(s): *Jiguang Sun, *Michigan Technological Univers*.

The quad-curl problem arises in the study of the electromagnetic interior transmission problem and magnetohydrodynamics (MHD). In this talk, we study the quad-curl eigenvalue problem and propose a mixed method using edge elements. Assuming stringent regularity of the solution of the quad-curl source problem, we prove the convergence and show that the divergence- free condition can be bypassed.

14th U.S. National Congress on Computational Mechanics
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Title: Large and Fast Density Functional Theory Calculations

Author(s): *Phanish Suryanarayana, *Georgia Institute of Technology*.

Electronic structure calculations based on Density Functional Theory (DFT) have been remarkably successful in describing material properties and behavior. However, the large computational cost associated with these simulations has severely restricted the size of systems that can be routinely studied. In this talk, previous and current efforts of the speaker to develop efficient real-space formulations and parallel implementations for DFT will be discussed. These include linear scaling methods applicable to both insulating and metallic systems.

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Title: Particle-Based Modeling of Clothes Washing and Drying Process

Author(s): *Masaaki Suzuki, *Tokyo University of Science*; Hiroshi Okuda, *The University of Tokyo*.

In recent years in the Japanese washing machine market, demand for high-performance washing and drying machines is increasing. Since it is difficult to further enhance the functionality of the product simply by trial and error using the actual machine, support for design and development by numerical simulation is required. Numerical analysis that uses heat balance and mass balance as a basic formula has been studied well for drying phenomena so far, and analysis examples for drum-type dryers are also available. However, such an approach does not address the dynamic behavior of clothes in the drum. In this research, we develop a particle-based simulation model for numerical analysis of washing and drying process of multiple clothing, which are flexible objects. A mass-spring-damper system is used to model cloth. Particularly, in order to evaluate the degree of wrinkle, connect particles (mass points) with a composite element combining multiple springs and dampers. For fluids, pressure and volume are modeled by repulsive forces acting on the particles according to the distance between the particles. Also, the viscous force is modeled by a force proportional to the speed difference with neighboring particles. In the drying process, the drying rate, that is, the decreasing rate of the moisture content of the clothes, is considered to be influenced by the shape and movement of the fabric in addition to the relative humidity of the outside air. In order to model the drying process, the moisture content is defined for each cloth particle and its temporal change is expressed by the formula in which the influence of cloth shape and motion are both described as inhibiting factors of drying. Conversely, a change in moisture content affects the structural and dynamic properties of the fabric. To consider the coupling between drying process and kinetics of clothes, we focus on fabric mass and flexural rigidity, and decrease mass and increase bending spring strength with decreasing moisture content. As a numerical experiment, simulations of the cloth in the fluid were executed in order to evaluate the influence of the difference in drum angle on cleaning ability. As an index of cleaning ability, external force applied to cloth particles was observed. As a result, it was found that the average external force is the largest when the drum angle is 45 degrees, and decreases as the angle increases or decreases from 45 degrees.

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Title: A Concurrent Coupling of Peridynamics and Classical Continuum Mechanics

Author(s): Xiaonan Wang, *UNCC*; *Alireza Tabarraei, *UNCCa*.

A problem of significant importance in solid mechanics is the accurate modeling of fracture. Several numerical techniques have been developed in the past for treating discontinuities and predicting crack growth. More recently, fracture modeling techniques based on peridynamics nonlocal continuum theory have been developed. In peridynamics, the forces acting at a particle are obtained by an integral operator that sums pairwise internal forces exerted on the particle by all the particles located at a finite distance from the particle of interest. In contrast to classical continuum theory, peridynamics theory does not make any assumption on the differentiability of displacement field for obtaining the forces. The main advantage of peridynamics is that no assumption is made on the continuity of the displacement field hence discontinuity in the displacement field due to the presence of cracks does not necessitate special treatments. Peridynamics performance has been validated by applying it to several sophisticated applications including polycrystals fracture, fracture of composite materials, structure stability and failure analysis, modeling of structure response under extreme loading, material fragmentation under impact dynamic fracture analysis, simulation of the kinetic of phase transformation and modeling heat transition in bodies with evolving cracks. In addition to the numerical verifications, rigorous mathematical analysis have been used to examine the properties of peridynamics. Although the peridynamic theory is capable of modeling damage formation and growth without resorting to any external criteria, numerical simulations using peridynamics are computationally expensive. The high computational cost is attributed to the nonlocality of the theory. In nonlocal theories each particle interacts with a large group of particles, resulting in costly assembly operations of the nonlocal discrete systems. Another issue associated with peridynamics is the prescription of displacement and traction boundary conditions. Since the variation formulation of the peridynamics does not include tractions, the forces acting on the surface are prescribed as body forces acting within a _ctitious boundary layer under the surface. Similar to tractions, displacements boundary conditions are imposed by constraining the displacement of material points within a fictitious boundary layer. A linear interpolation is used to approximate the value of the displacement of material points in the boundary layer based on the boundary conditions and the displacement of the points within the domain. The inaccuracy in prescribing the boundary conditions in peridynamics reduces the accuracy of modeling predictions. In this paper, we propose a technique for coupling peridynamics with classical continuum mechanics for dynamic fracture modeling. In our proposed coupling technique, peridynamics description is used only in the areas of the domain where nucleation or growth of discontinuities is probable, and classical continuum mechanics is used elsewhere. Therefore, fine scale behavior is captured by the peridynamics zone and finite elements are used in the zones where solution is smooth. The proposed method takes advantages of the salient features of both techniques i.e. straight forward application of boundary conditions along with lower computational cost of classical continuum mechanics and peridynamics superiority in fracture simulation. Our proposed coupling method is based on the Arlequin scheme and employs Lagrange multipliers to enforce displacement compatibility between peridynamics and classical continuum mechanics. We present a novel technique for removing the issue of spurious wave reflections at the interface of classical continuum mechanics and peridynamics.

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Title: In Situ Intra-Bundle Full Field Measurement in a Single Carbon Fiber Bundle Composite under Transverse Load

Author(s): *Ilyass Tabiai, Martin Lévesque, *École Polytechnique Montréal*; Damien Texier, *Ecole de Technologie Superieur*; Daniel Therriault, *Ecole Polytechnique de Montral*.

The peridynamic (PD) theory has been proposed to overcome modeling difficulties related to initiation and growth of multiple discontinuities in fibre reinforced composites (FRCs). Full field measurements of displacement and deformation during damage (discontinuities) were not found to be available in the literature. The purpose of this work is thus to provide quantitative experimental data in the vicinity of a fiber inside a bundle during damage in order to compare such results with PD simulation results. A confocal laser microscope is used to analyze an in-situ quasi-static test of a single bundle of carbon fibers embedded in a standard dog-bone specimen under transverse load. Crack initiation and propagation are observed. Digital Image Correlation (DIC) analysis is then used to provide precise measurements of displacements, strains and out-of-plane displacements until specimen failure. DIC analysis requires an additional layer of material (paint or particles) at the observed specimen surface to form a random speckle pattern which is used to track each material point; for this work, no additional material was used to create a speckle pattern since the material's roughness is used for tracking purposes. This improvement allows to reach a higher accuracy overall but specifically in interfaces and cracks' vicinity. The material analyzed here is a dogbone specimen made out of epoxy with a single bundle of carbon fibers under transverse load. Results presented reveal strain and displacement levels during damage initiation and propagation inside and in the vicinity of a bundle of carbon fiber. High strain levels are measured around each single fiber and the whole bundle. Impact of crack initiation and propagation on the strain field will be presented. The method is shown to be promising in order to provide quantitative data about FRCs' damage. Such results can then be compared with simulation methods allowing for initiation and propagation of discontinuities in a non-homogeneous media to better model damage of FRCs.

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Title: Coupled Continuum-Atomistic Simulations of Incommensurate to Commensurate Transformations in Twisted Graphene Bilayers

Author(s): Kuan Zhang, *Ellad Tadmor, *University of Minnesota*.

The synthesis of graphene, a one-atom thick 2D graphitic sheet, was a revolution in materials physics. Since then a host of other 2D materials have been discovered that can be stacked to create layered heterostructures with remarkable properties. Due to the weak van der Waals interaction between layers, the resulting structures can be incommensurate and therefore challenging to model. We describe recent work on developing a hybrid continuum-atomistic computational framework for simulating the mechanical response of 2D heterostructures. In agreement with experiments, simulations of twisted bilayer graphene show a transformation from an initially incommensurate structure to commensurate structures separated by localized solitons. This behavior is explained using a simple mechanical model.

14th U.S. National Congress on Computational Mechanics
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Title: Multiscale Modeling of Dislocation Kinetics in BCC Iron

Author(s): *Akiyuki Takahashi, Kazuki Takahashi, *Tokyo University of Science*.

The dislocation behavior in BCC metals is known to be quite complex due to a strong dependence of dislocation behavior on the dislocation character, such as edge, screw and mixed character. The dislocation dynamics (DD) simulation is now becoming a powerful simulation tool for investigating the plastic deformation of metals based on the collective behavior of discrete dislocations. However, for simulating the plastic deformation of BCC metals with such a complex dislocation behavior, the precise model of dislocation kinetics must be established and implemented into the DD code. This paper presents the molecular dynamics (MD) modeling of dislocation kinetics in BCC iron and the application of the model to the DD simulations for predicting the plastic deformation of BCC iron. In the MD modeling, the dislocation core structures of not only edge and screw and also mixed dislocations are first analyzed. Then, the relationship between the atomistic dislocation core structure and the dislocation kinetics is investigated. By simulating a simple dislocation behavior under applied shear loadings, dislocation mobility, which is the sensitivity of dislocation velocity to the applied shear stress, is modeled in a wide range of temperature conditions. By fitting the numerical results of dislocation mobility, an equation approximating the dependence of dislocation mobility on the dislocation character is derived. The dislocation mobility equation is then implemented into the DD simulation code. Using the DD code, dislocation source behavior in BCC iron is simulated, and the numerical result is compared to an available experimental picture for validating the modeling of dislocation kinetics.

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Title: Porous Composite with Negative and Positive Thermal Expansion Obtained by Multi-Material Topology Optimization and Additive Manufacturing

Author(s): *Akihiro Takezawa, *Hiroshima university*; Makoto Kobashi, *Nagoya university*.

To realize negative thermal expansion (NTE), porous composites made of two materials with different coefficients of thermal expansion are being actively researched. NTE can be realized by taking advantage of the thermal deformation mechanisms of a composite's internal geometry. However, the ability to tune thermal expansion is desirable not only to make it negative. Designing a material with arbitrary thermal expansion, including positive thermal expansion, using these phenomena extends the material's applications. Also, additive manufacturing (AM) could provide a new way to fabricate composites by layering multiple materials on arbitrary points in three-dimensional space. In this study, we developed a porous composite with arbitrary thermal expansion, including negative and positive thermal expansion as well as isotropic and anisotropic thermal expansion, by using multi-material photopolymer AM. The internal geometries producing such characteristics were designed by topology optimization, which is the most effective structural optimization method both in realizing macroscopic inward deformation and in maintaining stiffness. The designed structures were converted to three-dimensional models and fabricated by multi-material photopolymer AM. Using laser scanning dilatometry, we measured the thermal expansion of these specimens, revealing well-ordered thermal expansion, from anisotropic positive thermal expansion to anisotropic negative thermal expansion.

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Title: Uncertainty Quantification in Composite Woven Materials Using a Statistically Equivalent Representative Volume Element with Discrete Defects

Author(s): *David Tal, Jacob Fish, *Columbia University*.

The random nature of the micro-structural attributes in fabricated composite material gives rise to quantifying material uncertainty and developing a representative volume element which incorporates the aforementioned randomness. The material uncertainty is quantified using a methodology for generating a realistic volume element with discrete defects that are statistically equivalent to random defects structure. Experimental data extracted from cross-sectional micro-graphs leads to the geometric statistical characterization of stochastic micro-scale discontinuities. Three dimensional discrete ellipsoidal voids are then introduced to a defect-free eight harness weave model based on the obtained statistical characteristics, using a Monte-Carlo simulation. The geometric parameters of the generated defects result in target statistics equivalent to that of the defects in the micro-graphs.

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Title: A Discontinuous Galerkin / Cohesive Zone Model Approach to Simulating Dynamic Fracture in Very Large Shell Structures

Author(s): *Brandon Talamini, Raul Radovitzky, *MIT*.

Fracture is often a critical concern in the design of large-scale, thin structures such as aircraft fuselages, ship hulls, and automobiles, which has spurred the development of numerous numerical shell fracture techniques in the last 10-15 years. Resolving the fracture process in full-scale shell structures often exceeds the computing power of single workstations and demands parallel computation. At the same time, shell fracture interacts with other strongly nonlinear phenomena, including buckling, wrinkling, and inelastic material behavior, which must be captured to make useful predictions. In this work, we propose a computational framework for the simulation of deformation and fracture in shells that addresses these challenges. Spatial discretization of the shell is accomplished with a new discontinuous Galerkin (DG) method for nonlinear shear-flexible (Reissner-Mindlin) shell theory. The DG method alleviates shear locking in a natural way, without recourse to reduced integration schemes or mixed variational methods. As a practical consequence, the method can be cast in terms of a discrete energy minimization principle, which guarantees symmetry of the stiffness matrix and opens the door to applying powerful tools of mathematical optimization for solution. As a further benefit, resolving locking through the DG approach means that standard Lagrange polynomials can be used as basis functions, which simplifies the formulation in the case of large deformations and finite rotations. Fracture is modeled using interface elements and a specialized shell cohesive zone model of fracture phrased directly in terms of stress resultants. This shell DG/interface element methodology inherits the scalability properties demonstrated previously for fracture in solids, while avoiding artificial elastic compliance issues that are common in other cohesive model approaches. A key feature of the framework is the capability to model the effect of through-thickness shearing on fracture, thanks to the shear-flexible shell theory and the careful construction of the cohesive zone theory. We show that this is especially important for impulsive loading conditions, where shear-off failure near stiffeners and supports is common. We illustrate the ability of the framework to capture realistic deformations and fracture modes for thin structures through numerical examples, and demonstrate the parallel computation capabilities of the method through the simulation of explosive decompression of the skin of a full-scale passenger aircraft fuselage.

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Title: A Homogenized Gradient Elasticity Model for Plane Wave Propagation in Bi-Laminate Composites

Author(s): *Swee Hong Tan, Leong Hien Poh, *National University Singapore*.

Wave dispersion occurs when propagating through a heterogeneous medium. Such a phenomenon becomes more pronounced when the smallest wavelength of the incoming pulse approaches the size of a unit cell, as well as when the contrast in the mechanical impedance of the constituent materials increases. In this contribution focusing on composite laminates, we seek an accurate description of the wave propagation behavior without the explicit representation of the underlying constituent materials. To this end, a gradient elasticity model based on a novel homogenization strategy is proposed. The intrinsic parameters of the gradient enhanced continuum capturing the underlying micro-inertia effects and nonlocal interactions, are fully quantified in terms of the constituent materials' properties and volume fractions. The framework starts with suitable kinematic decompositions characterizing a unit cell. The Hill-Mandel Principle is next applied to consistently translate the energy statements from micro to macro. The predictive capability of the proposed model is demonstrated through four benchmark examples encompassing a comprehensive range of material properties and volume fractions.

14th U.S. National Congress on Computational Mechanics
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Title: An Absorbing Boundary Condition to Minimize Wave Reflection in Atomistic Simulations

Author(s): A.V. Rammohan, *Vincent Tan, *National Univ of Singapore*.

Computer-based simulations are frequently used to ascertain the response of materials to different loading scenarios. Such simulations (for instance, using atomistic dynamics codes) would in principle require the specimen to be of infinite size in order to completely eliminate the effect of its boundary on the solution at the location of interest. However, simulations on infinite or very large domains (that is, comprising a very large number of atoms) imply exorbitant computational costs and are therefore often unfeasible. A common solution is to truncate the domain at a location sufficiently far away from the region of interest and then restrict the simulation to the internal atoms [1]. However, if left untreated, the artificially introduced boundary region may itself lead to aberrant behavior, a paradigmatic example of which is the nonphysical reflection of waves incident at the boundary. In this work, we derive and demonstrate from first principles a simple yet effective solution to mitigate the manifestation of such spurious wave reflections at the surface of an artificially truncated domain. We obtain an explicit relationship between the displacement and the velocity terms of the terminal atom and the additional force that needs to be applied on this atom in order to absorb any incident wave. Furthermore, we demonstrate that modifying the terminal atom by halving its mass results in a qualitative change in the relationship in that the force ceases to be dependent on the displacement of the terminal atom. Lastly, we show how, as the wavelength of the incident wave increases vis-à-vis the interatomic spacing, the relationship simplifies to a form that is well-known in continuum-based [2] and multiscale contexts [3], thus providing an analytical basis for choosing optimal parameters. A numerical example demonstrates the implementation and efficacy of this method. Our findings will be of interest not only to researchers performing numerical simulations on artificially truncated domains, but also to those working in multi-scale simulations where similar spurious wave reflections occur at the atomistic-continuum interface. References [1] D. Givoli, Numerical Methods for Problems in Infinite Domains, Elsevier, 2013. [2] J. Achenbach, Wave Propagation in Elastic Solids, Elsevier, 2012. [3] S. Qu, V. Shastry, W.A. Curtin, R.E. Miller, A finite-temperature dynamic coupled atomistic/discrete dislocation method, Model. Simul. Mater. Sci. Eng. 13 (2005) 1101–1118. doi:10.1088/0965-0393/13/7/007.

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Title: An Absorbing Boundary Condition to Minimize Wave Reflection in Atomistic Simulations

Author(s): A.V. Rammohan, *Vincent Tan, *National Univ of Singapore*.

Computer-based simulations are frequently used to ascertain the response of materials to different loading scenarios. Such simulations (for instance, using atomistic dynamics codes) would in principle require the specimen to be of infinite size in order to completely eliminate the effect of its boundary on the solution at the location of interest. However, simulations on infinite or very large domains (that is, comprising a very large number of atoms) imply exorbitant computational costs and are therefore often unfeasible. A common solution is to truncate the domain at a location sufficiently far away from the region of interest and then restrict the simulation to the internal atoms [1]. However, if left untreated, the artificially introduced boundary region may itself lead to aberrant behavior, a paradigmatic example of which is the nonphysical reflection of waves incident at the boundary. In this work, we derive and demonstrate from first principles a simple yet effective solution to mitigate the manifestation of such spurious wave reflections at the surface of an artificially truncated domain. We obtain an explicit relationship between the displacement and the velocity terms of the terminal atom and the additional force that needs to be applied on this atom in order to absorb any incident wave. Furthermore, we demonstrate that modifying the terminal atom by halving its mass results in a qualitative change in the relationship in that the force ceases to be dependent on the displacement of the terminal atom. Lastly, we show how, as the wavelength of the incident wave increases vis-à-vis the interatomic spacing, the relationship simplifies to a form that is well-known in continuum-based [2] and multiscale contexts [3], thus providing an analytical basis for choosing optimal parameters. A numerical example demonstrates the implementation and efficacy of this method. Our findings will be of interest not only to researchers performing numerical simulations on artificially truncated domains, but also to those working in multi-scale simulations where similar spurious wave reflections occur at the atomistic-continuum interface. References [1] D. Givoli, Numerical Methods for Problems in Infinite Domains, Elsevier, 2013. [2] J. Achenbach, Wave Propagation in Elastic Solids, Elsevier, 2012. [3] S. Qu, V. Shastry, W.A. Curtin, R.E. Miller, A finite-temperature dynamic coupled atomistic/discrete dislocation method, Model. Simul. Mater. Sci. Eng. 13 (2005) 1101–1118. doi:10.1088/0965-0393/13/7/007.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Inverse Monte Carlo Grain Growth Analysis for Process Design

Author(s): *Yixuan Tan, *Rensselaer Polytechnic Institu*; Antoinette Maniatty, John Wen, Chengjian Zheng, *RPI*.

In this work, we solve the inverse problem to determine the required processing conditions to create a prescribed columnar microstructure in a metal film. Thermal processing is used by metals manufacturers to generate desired microstructural features and thus, properties. However, the processing conditions are typically specified based on experience and trial and error, leading to a longer development cycle and resulting process parameters that may not be optimized. In this work, we develop an approach to determine the processing parameters that will create a columnar grain structure. The columnar grain structure results from a slowly moving temperature gradient applied to the metal, and creates a creep resistant material along the elongated grain direction. To model the forward problem, we developed a new parallel Monte Carlo method for modeling microstructure evolution in manufacturing processes that involves a time-dependent local temperature gradient. To capture the effects of the temperature gradient, the site selection probability in each Monte Carlo step is biased accordingly across the domain. This new biased sampling strategy is built upon the scaling relation between the Potts Monte Carlo method and physical observations. The inverse problem of determining the process parameters to create a columnar microstructure is posed as a binary classifier. To improve the computing performance, a reduced model or classifier is built from the new Monte Carlo method, and it is used as the forward model in the inverse problem. The forward grain growth model takes as inputs the temperature field calculated by a heat transfer finite element model. A genetic algorithm is used to drive the heat transfer model and the forward grain growth model to search for the optimal process parameters under constraints such that columnar growth can be created. The manufacturing design parameters that control the temperature field are solved for in this inverse analysis. Some examples demonstrating the algorithm will be presented.

14th U.S. National Congress on Computational Mechanics
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Title: Matching Boundary Conditions for a Heterogeneous Atomic Chain

Author(s): *Shaoqiang Tang, *Peking University*; Xingru Chen, *Dartmouth College*; Shuyu Liu, *Johns Hopkins University*.

We propose accurate boundary treatments for a heterogeneous atomic chain, in terms of matching boundary conditions (MBC). The main challenge lies in reproducing the physical reflection across the boundary to a correct amount. With reflection coefficients we demonstrate that the accuracy improves when more atoms are used in the boundary condition. The inclusion of an atom in the embedded sublattice B may considerably enhance the performance. Numerical test illustrates the effectiveness of the proposed MBCs. Extensions to two dimensional lattices will also be discussed, which has potential applications in twin boundaries.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Fluid-Structure Interaction Model of Human Phonation

Author(s): *Pooya Tavakoli-saberi, Prof.luc Mongeau, *McGill University*.

Phonation involves the interaction between the airflow through the glottis and the vocal folds' deformations. Computer simulations provide useful insight into the mechanics of the self-oscillations. Patient specific models can be used to develop treatment methods and to help physicians predict possible outcomes. The goal of the present study was to develop a model to evaluate internal stresses and strains within different types of tissues, understand the effects of changes in vocal folds' material properties and the corresponding frequency of oscillation. In the current work, a 2.5D (one element thick) Fluid Structure Interactions (FSI) model of human phonation was created using ANSYS. The fluid flow in the glottis was modeled as a compressible ideal gas with deforming mesh. The trans-glottal pressure gradient was varied as a parameter. The solid domain, i.e. the vocal fold tissue, was modeled as a three-layer viscoelastic material with large deformations and non-rigid boundary conditions. A cavity filled with a synthetic scaffold material was added to simulate the presence of an injectable composite hydrogel. The three layers consisted of the epithelium, the Basement Membrane Zone (BMZ) and the Lamina Propria (LP). The complex unsteady flow was then solved using ANSYS Fluent, coupled to the ANSYS Mechanical Finite Element solver visa the ANSYS System Coupling Module where the pressures forces and mesh displacements on the fluid-structure interfaces are coupled at each iteration. The generated data was then compared with experimental data from the perfusion bio-reactor developed by Latifi et al [1]. The primary results calculated stresses in the range of 500-1000 kPa which is commonly observed in the vocal folds' tissues [1]. The data also provided a frequency of vibration similar to experimental observations [2]. The influence of scaffold rigidity on the model vibration characteristics was investigated to determine whether variations in scaffold composition during tissue reconstruction could be detected from macroscopic changes in phonation output. [1] Latifi, Neda, Hossein K. Heris, Scott L. Thomson, Rani Taher, Siavash Kazemirad, Sara Sheibani, Nicole Y.k. Li-Jessen, Hojatollah Vali, and Luc Mongeau. "A Flow Perfusion Bioreactor System for Vocal Fold Tissue Engineering Applications." Tissue Engineering Part C: Methods 22.9 (2016): 823-38. Web. [2] Sundberg, Johan, Ronald Scherer, Markus Hess, Frank Müller, and Svante Granqvist. "Subglottal Pressure Oscillations Accompanying Phonation." Journal of Voice 27.4 (2013): 411-21. Web.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Segmentation of Atherosclerotic Plaques in MR Carotid Artery Images

Author(s): *Joao Tavares, Danilo Jodas, *FEUP*; Aledir Pereira, *UNESP*.

Abstract The composition of atherosclerotic plaques in the carotid artery plays an important key to determine their evolution and, consequently, the risk of reduction/obstruction of the blood flow through the artery. Computational algorithms have been proposed in many studies to segment, i.e. to identify [1], and assess atherosclerotic plaques and their main components in images [2]. The use of such algorithms allows, for example, the evaluation more efficiently of the risk to cerebral events. The aim of this work was the development of an algorithm to segment atherosclerotic plaques and the related main components in MR images of the carotid artery, which has two main steps: 1) segmentation of the lumen and arterial walls and 2) further segmentation of the atherosclerotic plaques. The first step provides the region containing the atherosclerotic plaques, i.e. the region between the lumen and arterial wall boundaries. In this step, the K-means algorithm is used to obtain the regions comprised by the pixels of low intensity and related to the lumen and the background of the image under analysis. Since the lumen region is approximately circular, indexes of circularity and irregularity are used to find the desired region among the various region candidates. Then, a deformable level-set based model is used to refine the lumen boundary. Once the lumen is segmented, the final segmentation of the artery wall boundary is accomplished using also a deformable model. In the second step, the segmentation of the atherosclerotic plaques is performed by using a fuzzy C-means algorithm. Again, a deformable model is used to refine the boundaries of the segmented plaques. Besides the description of the developed algorithm, experimental results will be presented and discussed. Acknowledgements This work was partially funded by Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), funding agency in Brazil, under the first author's PhD Grant with reference number 0543/13-6. Authors gratefully acknowledge the funding of Project NORTE-01-0145-FEDER-000022 - SciTech - Science and Technology for Competitive and Sustainable Industries, cofinanced by "Programa Operacional Regional do Norte" (NORTE2020), through "Fundo Europeu de Desenvolvimento Regional" (FEDER). References [1] D.S. Jodas, A.S. Pereira, J.M.R.S. Tavares, A review of computational methods applied for identification and quantification of atherosclerotic plaques in images. Expert Systems with Applications, 46, 1-14, 2016. Z. Ma, J.M.R.S. Tavares, R.N. Jorge, T. Mascarenhas, A Review of Algorithms for Medical Image Segmentation and their Applications to the Female Pelvic Cavity, Computer Methods in Biomechanics and Biomedical Engineering, 13, 235-246, 2010.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Posteriori Error Estimation for Several Classes of Finite Difference Schemes

Author(s): *Simon Tavener, *Colorado State University*; Jehanzeb Chaudhry, *Univesity of New Mexico*; Jeb Collins, *West Texas A&M*; John Shadid, *Sandia National Laboratories*.

Finite difference schemes are a popular choice to solve both ordinary and partial differential equations. Examples include Adams Bashforth and Runga Kutta methods for solving systems of odes, IMEX schemes for parabolic and hyperbolic partial differential equations and the Lax Wendroff scheme for solving nonlinear conservation laws. Finite difference schemes are amenable to a posteriori error analysis if they can be recast into a suitable variational form and appropriate adjoint problems and (computable) residuals can be defined. We illustrate this approach for several common finite difference schemes and demonstrate the accuracy of the error estimates obtained. Further, the a posteriori analysis distinguishes errors arising from distinct types of approximation. This can motivate new integration schemes and we provide one example.

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Title: Nano-Motions of FePd Nanorobots Subjected to Applied Magnetic Field by Molecular Dynamics Mode

Author(s): *Minoru Taya, *University of Washington*; Takehiro Matsuse, *Shinshu University*.

Shrinkage and relaxation motions of flexible FePd nanohelix of FePd nanorobots are simulated by molecular dynamics (MD) model where FePd is paramagnetic shape memory alloy that can exhibit phase transformation accompanied with softening of the nanohelix under applied magnetic field (H-field). Two designs of FePd nanorobots are used; (i) FePd cylindrical head connected to FePd nanohelix tail, and (ii) FePd nanohelix alone. The geometry and dimensions of the FePd robots are taken after the as-processed FePd nanoorobots. In the MD simulation, FePd head and nanohelix are divided into a number of segmented FePd spheres, each having its magnetic moment. The magnetization – magnetic field (M-H) curve of a segmented sphere is based on the experimental M-H curve of FePd nanoparticles which follows the paramagnetic M-H curve of Lagenvin type. The MD model accounts for five forces, (1) Magnetic forces among segmented spheres between the FePd cylindrical head and nanohelix, (2) Magnetic forces among segmented spheres in the nanohelix only, (3) Mechanical forces among segmented spheres in the nanohelix by using the mechanical nanohelix energy (harmonic oscillator potential), (4) Repulsive forces between segmented spheres across two turns of nanohelix by using Lennard-Jones potential and (5) Viscous forces arising as a result of the motions of segmented spheres in viscous fluid. These five forces are incorporated into Newtonian equation which is solved in time-step wise manner. The results of the MD model reveal that upon applied constant magnetic field the initial gaps (g = 3nm) between adjacent turns of FePd nanohelix are closed, resulting in the total shrinkage (Stot) of 47 nm of the FePd nanorobot. The effects of applied H-field on Stot are examined, by using the MD model and the M-H curve of FePd fitted with Langevin type, resulting in the smaller applied magnetic field leading to the smaller Stot. The results of the MD model provides us with an effective tool in the analysis and design of new nanorobots based on paramagnetic shape memory alloy of FePd nanohelices that can exert dynamic vibrations on target cells under oscillating magnetic field.

14th U.S. National Congress on Computational Mechanics
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Title: Reliable Automated Simulation Technologies to Aid in Diagnosing and Treating Heart Disease

Author(s): *Charles Taylor, *HeartFlow, Inc*.

Patient-specific models of blood flow constructed from coronary CT angiography (cCTA) images and using computational fluid dynamics are transforming the diagnosis of heart disease by providing a safer, cheaper and more efficient procedure as compared to the standard of care that often involves nuclear imaging and invasive diagnostic cardiac catheterizations. Such image-based simulations require an accurate segmentation of the coronary artery lumen from cCTA images and leverage biologic principles relating form (anatomy) to function (physiology). Importantly, efficient mesh generation and computational methods are necessary to return results quickly enough to be compatible with clinical demands. HeartFlow has developed a non-invasive test, FFRCT, based on computed flow and pressure in the coronary arteries. FFRCT has been validated against invasive pressure measurements in more than 600 patients and demonstrated to improve care in numerous clinical studies to date. At present, FFRCT has been used for more than 10,000 patients in routine practice for clinical decision making in the United States, Canada, Europe, and Japan. Patient data is uploaded to the HeartFlow application running on Amazon Web Services, image analysis methods leveraging deep learning are used to create an initial patient-specific geometric model, sensitivity analysis is performed to assess the impact of image quality on geometric uncertainty and then a trained analyst inspects and corrects the patient-specific geometric model. Next fully-automated mesh generation techniques including anisotropic and boundary layer elements developed by Shephard and colleagues are used to discretize the model. Computational fluid dynamic analysis is performed on AWS to compute the blood flow solution. Results are returned to the physicians through a web interface or mobile application. New developments including the possibility of planning treatments and evaluating risk of rupture of coronary plaques will be discussed. The impact of automatic mesh generation techniques developed by Professor Mark Shephard on the field of image-based modeling will be described. [1] Taylor CA, Fonte TA, Min JK., Computational Fluid Dynamics Applied to Cardiac Computed Tomography for Noninvasive Quantification of Fractional Flow Reserve, J Am Coll Cardiol. 2013;61(22):2233-2241.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Estimating the Convergence of Apparent Properties and Maximum Response in Computational Homogenization

Author(s): *Kirubel Teferra, *US Naval Research Laboratory*; Lori Graham-Brady, *Johns Hopkins University*.

In this work, the challenge of efficiently determining the representative volume size in computational homogenization is addressed by exploiting the assumption that mechanical response quantities are statistically homogeneous and ergodic random fields. If both input uncertainty and output response quantities are described by second order random fields, meaning they are entirely described by their marginal probability density function and autocorrelation function, then an exact expression exists for the variance of the spatial average of a response quantity, while a quasi-exact closed form expression exists for the cumulative distribution function of the maximum value of the response quantity over a finite domain. The primary challenge, then, is to determine the autocorrelation function of the response quantity of interest. In the proposed computational homogenization, a Monte Carlo approach is used to empirically determine the properties of the second order random fields that sufficiently characterize the response. Once established, both the variance of spatially averaged quantities and the cumulative distribution function of the maximum value of response quantities as a function of domain size can be determined through simple numerical computations, and no additional finite element simulation is required. After presenting the formulation, the method is demonstrated both on a simple analytical one-dimensional bar model and on a more challenging example involving Monte Carlo simulation of crystal plasticity finite element models of a polycrystalline Nickel super alloy. The presentation concludes with an in-depth discussion of the results and identification of challenges limiting widespread applicability.

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Title: Data-Interactive Computational Materials Physics: Studies of Precipitate Morphology by a Combination of Experiment, Nonlinear Elasticity and Machine Learning

Author(s): *Gregory Teichert, Emmanuelle Marquis, Krishna Garikipati, *University of Michigan*.

We present a study of the morphology of Mg-Nd precipitates, driven by large data sets of energy computations for a range of geometry features and material parameters. The energy computations account for the eigenstrain in the precipitate and the interfacial energy. The values used for the interfacial energies and precipitate elasticity constants are calculated rather than observed, therefore the uncertainty associated with the calculation error is incorporated. The study is enhanced by training a deep neural network to the data to represent the energy surface. Predictions for the equilibrium precipitate shape for a given set of material parameters correspond to energy minima with respect to the geometry features. By comparing predictions to experimental data, we find that the precipitate shape is largely driven by seeking equilbrium with respect to the strain and interfacial energies.

14th U.S. National Congress on Computational Mechanics
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Title: Bayesian Methods to Capture Inherent Material Variability in Additively Manufactured Samples

Author(s): Francesco Rizzi, Brad Boyce, Reese Jones, Jakob Ostien, *Jeremy Templeton, *Sandia National Labs*.

Additively manufactured samples have demonstrated significant variability in both estimated yield strength and failure stress. This variability is inherent in the material behavior and significantly greater than the measurement uncertainty. Bayesian calibration of material models is an attractive approach in this case because it can quantify the accuracy of estimates of model parameters, but suffers from incorrectly attributing the variability to measurement error rather than aleatoric uncertainty. In this presentation, we explore various approaches to account for material variability within a Bayesian calibration of a J2 plasticity model. Experimental data is provided in the form of nearly 1000 tensile tests of an additively manufactured specimen from 8 different lots. The Young's modulus may be easily estimated from the data, so we focus on calibrating the yield strength and hardening modulus. We consider several forms of model error, including treating each point along the stress/strain curve as an i.i.d. sample of the response, as well as treating each test curve as a data point with a parameterized error model. While the mean-plus-uncertainty of the calibrated model encompasses the test data, a realization-to-realization comparison suggests the additive noise model does not account for the observed variability in a physically meaningful way. The primary cause is that the variability does not conform to a simple Gaussian description, and further is interpreted within the Bayesian framework as an estimate of the error in the measurement process. As a result, individual realizations from this model cannot be used as a material model in a mechanics code, and as additional data is added, the calibration process becomes increasingly certain of the model parameters even as the variability remains finite. As an alternative, we consider the Embedded Error Model (EEM) in which the model parameters are represented as polynomial chaos expansions (PCEs) such that the calibration is performed on the coefficients. In this approach, because uncertainty is inherent in the expansion, the coefficients converge to a model representation with finite variance. We will compare the results of the EEM to more traditional Bayesian calibration methods and explore the impact on different measurement error models within this framework.

14th U.S. National Congress on Computational Mechanics
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Title: Tools for Scalable, Parallel Simulation of Problems with Evolving Domains

Author(s): *Saurabh Tendulkar, Ottmar Klaas, Rocco Nastasia, Mark Beall, *Simmetrix Inc.*.

Evolving geometric domains appear in a variety of problems of interest including metal forming, additive manufacturing, ballistics and fracture mechanics. The scale of problems of interest today often requires that such simulations be done on parallel computers, thus that all steps in the simulation must scale well in parallel. To do this requires close coupling between the solver and the procedures to modify the mesh to account for geometry changes as well as mesh adaptivity procedures based on error indicators. In problems where the model geometry is complex with many thousands of entities, storing the entire geometric model on all processors does not provide memory scalability in parallel, and it becomes necessary to distribute the geometric model itself among the processors involved in the simulation. Simmetrix has developed tools and methods for parallel distributed geometry, mesh generation and mesh adaptation to support such evolving geometry problems. These methods will be described with particular emphasis on the support of evolving geometries on distributed memory parallel computers. Several applications of these methods to problems in which the geometry and mesh evolve will be demonstrated.

14th U.S. National Congress on Computational Mechanics
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Title: Thermo-Mechanical Coupled Numerical Material Testing for Polymeric Composite Materials

Author(s): *Kenjiro Terada, Seishiro Matsubara, Masayasu Kishi, Mayu Muramatsu, *Tohoku University*.

We present a method of thermo-mechanical coupled numerical material testing (NMT), applicable for two-scale computations for polymeric composite materials. The incremental variational formulation (IVF) [1] is employed to define the global and local inf-sup problems for thermo-mechanically coupled phenomena within a certain time interval, while two-scale convergence theory in the mathematical homogenization framework is applied to derive micro- and macro-scale incremental potentials. The key ingredient of the formulation is the introduction of equilibrated and external (non-equilibrated) temperature fields. It should be noted that the formulation not only has obvious variational structures but also ensures the thermodynamic consistency. In order to apply our framework to polymeric composite materials, we employed a modified version of the constitutive model of polymeric materials based on multi-mechanism theory [2], whereas inclusions are modeled by standard thermo-hyperelasticity. The constitutive model consists of rheology elements that represent hyper-viscoelastic and viscoplastic deformations along with kinematic hardening and is intended to capture not only temperature and deformation rate dependencies, but also the transition between glassy and rubbery material responses around glass-transition temperature. When incorporating the constitutive model into the present two-scale IVF, we assume that viscoelastic and viscoplastic pseudo dissipation potentials can be additively decomposed and that the standard procedure is applicable for viscoplasticity. Several numerical examples are presented to validate the performance of the proposed framework of NMT along with the employed constitutive model and demonstrate the two-scale thermos-mechanical coupled phenomena typified by stress-softening, strain recovery, and self-heating phenomena. We then perform two-scale thermo-mechanical coupled analyses for polymeric composite materials by solving the derived two-scale inf-sup problems to characterize the multiscale mechanical-thermal coupling behavior and discuss the role of the equilibrated or non-equilibrated temperature fields. References: 1. Q. Yang, L. Stainier and M. Ortiz, “A variational formulation of the coupled thermos-mechanical boundary-value problem for general dissipative solids”, Journal of the Mechanics and Physics of Solids, 54, 401-424 (2005) 2. V. Srivastava, S.A. Chester, N.M. Ames, L. Anand, “A thermos-mechanically-coupled large-deformation theory for amorphous polymers in a temperature range which spans their glass transition”, International Journal of Plasticity, 26, 1138-1182 (2010)

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14th U.S. National Congress on Computational Mechanics
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Title: Visualization of Vascular Injuries in Extremity Trauma

Author(s): *Joseph Teran, *UCLA*.

A tandem of particle-based computational methods is adapted to simulate injury and hemorrhage in the human body. In order to ensure anatomical fidelity, a three-dimensional model of a targeted portion of the human body is reconstructed from a dense sequence of CT scans of an anonymized patient. Skin, bone and muscular tissue are distinguished in the imaging data and assigned with their respective material properties. An injury geometry is then generated by simulating the mechanics of a ballistic projectile passing through the anatomical model with the material point method. From the injured vascular segments identified in the resulting geometry, smoothed particle hydrodynamics (SPH) is employed to simulate bleeding, based on inflow boundary conditions obtained from a network model of the systemic arterial tree. Computational blood particles interact with the stationary particles representing impermeable bone and skin and permeable muscular tissue through the Brinkman equations for porous media. The SPH results are rendered in post-processing for improved visual fidelity. The overall simulation strategy is demonstrated on an injury scenario in the lower leg.

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Title: Modeling and Simulation of Patched Structure under Low Velocity Impact Loading

Author(s): *Stephanie TerMaath, *University of Tennessee*.

Composite patches are adhesively bonded to a metallic structure (forming a patched structure) as a repair method to restore load-carrying capacity and damage tolerance to damaged components. Many parameters are critical to the performance of patched structure: amount and type of degradation in the composite structure, number and orientation of plies in the composite structure, thickness and condition of the metallic structure, constitutive properties of all three materials, quality of the bond surface, and the damage tolerance properties of the three materials, disbonds, load redistribution, and stresses induced at edge of composite patch. To ensure reliable and optimized patch design, it is imperative to understand the effects of the many input uncertainties and their interactions. Computational simulation provides an efficient method to explore the effects of these parameters with the damage tolerance space. A validated model of patched structure was been developed and validated to investigate damage tolerance in patched structure. This model is then used to investigate the damage tolerance under low velocity impact - a common loading condition that can cause internal damage that is not visible during inspection. The model captures multiple damage modes, including metal damage, disbond at the metal/composite interface, delamination between composite layers, and composite damage. Model development and sensitivity analysis results will be presented. This high fidelity model that captures multiple damage mechanisms providing a method to characterize and optimize the damage tolerance space in terms of design and loading input parameters.

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Title: An Inverse Finite Element Method Based on Refined Zigzag Theory for Structural Health Monitoring of Laminated Composite and Sandwich Shell Structures

Author(s): Adnan Kefal, Erkan Oterkus, *University of Strathclyde*; *Alexander Tessler, *NASA Langley Research Center*.

The technology called structural health monitoring (SHM) is aimed at providing real-time information concerning structural condition and performance, and has many industrial applications. SHM is envisioned to increase human and environmental safety and permits the reduction in economic losses. A key component of SHM is real-time computation of structural deformations and stress states (known as shape and stress sensing) that can be achieved using a network of in-situ strain sensors aided by a suitable mechanics-based computational algorithm. One of the most robust and general algorithms for this purpose is known as the inverse finite element method (iFEM), which has been studied extensively over the past fifteen years [1]. In this paper, the iFEM formulation incorporates the kinematics of the refined zigzag theory (RZT), thus allowing highly accurate shape and stress sensing to be performed on laminated composite and sandwich plates and shells. The present iFEM formulation minimizes a weighted-least-squares functional that uses the complete set of strain measures of RZT via a three-node, C0-continuous inverse-shell element. By taking advantage of a robust weighting-coefficient modelling strategy only a relatively small number of strain gauges is required. This formulation can more accurately sense the deformed shape and stress distributions of thin, moderately thick, and thick shells than the previously developed formulation [2]. Two numerical example problems are examined: (1) a simply supported rectangular laminated composite plate, and (2) a wedge structure with a hole near one of the clamped ends. The numerical results demonstrate the superior capability and potential applicability of the present methodology for performing accurate shape and stress sensing of complex composite structures. References [1] Tessler, A. and Spangler, J. L., (2005). A least-squares variational method for full-field reconstruction of elastic deformations in shear-deformable plates and shells. Computer. Methods Appl. Mech. Engrg. 194, 327-329. [2] Cerracchio, P., Gherlone, M., Di Sciuva, M., and Tessler, A. (2015). A novel approach for displacement and stress monitoring of sandwich structures based on the inverse finite element method. Composite Structures, 127, 69-76.

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Title: Large-Scale Deterministic Inversion and Bayesian Calibration in Land-Ice Modeling

Author(s): *Irina Tezaur, John Jakeman, Mauro Perego, *Sandia National Laboratories*; Stephen Price, *Los Alamos National Laboratory*.

Mass loss from the polar ice sheets is expected to have a significant contribution to future sea-level changes. Predictions of ice sheet evolution are fraught with uncertainty, which comes from a number of sources, including poorly known model parameters, incomplete knowledge of ice-sheet initial and boundary conditions, uncertain future climate forcing, and sparsity/imprecision of observational data used to constrain ice sheet models. This talk will describe some of our work in quantifying uncertainties in ice sheet model inputs, in particular initial and boundary conditions, using formal methods of optimal parameter estimation and uncertainty quantification (UQ), in conjunction with computational tools that orchestrate these methods. After describing our project for land-ice modeling, known as PISCEES (Predicting Ice Sheet Climate Science Evolution at Extreme Scales) and our FELIX (Finite Elements for Land Ice eXperiments) land-ice simulation tool, we will detail the “end-to-end” workflow we have developed to provide probability distribution functions (PDFs) on ice sheet model outputs of interest (e.g., ice sheet mass loss over time). This workflow consists of three stages: (1) deterministic inversion, (2) Bayesian calibration, and (3) forward propagation of uncertainty. To remain within the scope of this minisymposium, attention is focused on the first two stages. Specifically, we will discuss approaches for estimating the basal friction coefficient, an important high-dimensional parameter used to define the initial and boundary conditions in ice sheet models, under the presence of uncertainty. First, we will describe our approach for inverting for the basal friction by solving a large-scale partial differential equation (PDE)-constrained optimization problem that minimizes the model mismatch with observations of surface ice properties (e.g., surface velocity, surface mass balance). We then turn our attention to solving this inverse problem in a Bayesian setting, that is, determining the PDF of the basal friction given uncertainties, e.g., measurement error or noise, in the observed quantities. Our deterministic optimization is consistent with its Bayesian analog: it is used to find the MAP point of the posterior distribution. To address the challenge of the curse of dimensionality in the Bayesian inverse problem, we assume our posterior PDF is a Gaussian whose covariance is the square root of an elliptic partial differential equation, namely a low rank Laplace approximation, where the rank is the number of directions (linear combinations of the parameters) that informed directions of the posterior. We present results of the proposed inversion/calibration approaches on several Greenland ice sheet problems with varying resolutions.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: U-Splines: Splines over Unstructured Meshes

Author(s): *Derek Thomas, Kevin Tew, *Coreform LLC*; Michael Scott, *Brigham Young University*.

We present motivation and results for algorithms to construct spline basis functions over unstructured quad meshes that allow for the presence of T-junctions between mesh faces. We focus particularly on the requirement of local linear independence of the basis functions. Our construction overcomes the analysis-suitability constraints that have been established for T-splines. We also consider the inclusion of extraordinary points in the mesh.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Buckling Behaviour of Thin Walled Composite Box Beams with Variable Stiffness

Author(s): Muhsin Gökhan Gunay, *Taner Timarci, *Trakya University, Edirne*.

Buckling of thin walled composite laminated box beams with variable stiffness is investigated in this study. The analytical model developed accounts for flexural-torsional coupling and warping effects as well as the variable stiffness along the contour of the cross section of the beam. The variable stiffness is acquired by constructing laminates with curvilinear fibers having certain specific paths. The orientation of fibers varies by depending on the fiber path along the contour of the cross-section in each layer. Governing equations of buckling behaviour are derived by use of Hamilton's principle. A displacement based finite element method is used to solve the analytical model and to predict critical buckling loads and corresponding modes. Numerical results are obtained for different fiber paths and lay-up configurations and compared with the solutions of the available finite element analysis softwares using shell element.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Quantitative Prediction of Epitaxial Columnar Grain Texture from Process Parameters in Metal Additive Manufacturing

Author(s): *Albert To, Jian Liu, Erica Stevens, Markus Chmielus, *University of Pittsburgh*.

Metal additive manufacturing (AM) such as laser directed energy deposition (DED) has the powerful capability to produce very different microstructural features hence different mechanical properties in metals using the same feedstock material but different values of process parameters. However, the relation between processing-microstructure is investigated mostly by experiments so far, which is expensive and time-consuming since the parameter space is quite large. The lack of a reliable theoretical model of the processing-microstructure relationship of AM material is preventing AM technology from being widely adopted by the manufacturing community. Hence, the goal of this work is to establish the link between the microstructure (texture) and the process parameters (laser power, scanning speed, preheat and scanning strategy) of a metal AM process. To achieve the above goal, a quantitative method based on the epitaxial growth of columnar grains within and across melt pools is proposed to predict the texture formation during a metal AM process. Both analytical modeling and FEM simulation have been used to predict the geometry and thermal profile of the quasi-steady melt pool. The thermal gradient distribution within the 3D melt pool determines the crystallography direction and growth direction of the columnar grains within each deposited single tracks. For a bulk part with multiple tracks and layers, the epitaxial growth of grains across melt pools of neighboring tracks also affect the grain growths and texture formulation. The single tracks with the predicted geometry are amalgamated together to represent the bulk part, and the epitaxial growth of grains across the boundary of neighboring tracks are quantitatively modeled. The effect of overlapping between the tracks (hatching space) and layers (layer thickness) and the rotation of tracks (scanning strategy) is hence accounted for. The proposed method is calibrated and validated by experimental studies of Inconel 718 on a laser DED system (LENS 450). The printing and the EBSD characterization of both single tracks and multi-layer bulk parts are performed. The predicted texture has been shown to have similar patterns and intensities to that obtained from the experiments using the same process parameter values and scanning strategies.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Radiation Hydrodynamics with High-Order Finite Elements in the BLAST Code

Author(s): Robert Anderson, Thomas Brunner, Veselin Dobrev, Tzanio Kolev, Robert Rieben, *Vladimir Tomov, *LLNL*.

BLAST is a multi-material arbitrary Lagrangian-Eulerian (ALE) code based on high-order finite elements [1,2]. We present our discretization method for coupling hydrodynamics to grey radiation diffusion. The method supports materials with non-trivial equations of state and each material can have a distinct temperature-dependent opacity model. In space, the radiation hydrodynamics system is discretized by a mixture of high-order H1 (mesh position, velocity), discontinuous L2 (material energies, radiation energy) and Hdiv (radiation flux) finite element spaces. Because the small radiation diffusion time scales require implicit evolution of the radiation variables, we derive an IMEX time integration scheme that blends explicit hydrodynamics and implicit diffusion sub-steps. Using a smooth manufactured solution, we show that the method is second order in space-time, for both thin and thick regimes, and conserves total energy. Every implicit radiation diffusion step requires solving a nonlinear system. One way we solve its Jacobian is to reduce it to a global H(div) system for the radiation flux, and then recover the radiation and material energies by back-substitution. We also present a different approach, based on a two-block overlapping Gauss-Seidel iteration. The first block couples material energies to radiation energy, and is solved locally. The second block leads to a global H(div) system, which, in the future multigroup case, is solved independently for the radiation flux of every group, thus avoiding the H(div) coupling between groups. We present results obtained by both methods on standard radiation diffusion benchmarks. During the remap phase of the ALE method, transfer is performed only for the radiation energy field. Its resulting gradient is then used to approximate the radiation flux on the new mesh. We show ALE results for the radiating Kelvin-Helmholtz instability test, followed by a more challenging ICF capsule simulation (originally proposed by R. Tipton), where a four-pulse radiation temperature drive compresses a deuterium capsule. [1] High-Order Curvilinear Finite Element Methods for Lagrangian Hydrodynamics, V. Dobrev, T. Kolev, R. Rieben, SIAM JSC 34, B606–B641. [2] Multi-material closure model for high-order finite element Lagrangian hydrodynamics, V. Dobrev, T. Kolev, R. Rieben, V. Tomov, IJNMF 82(10), 689-706. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, LLNL-ABS-725123

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Theoretical and Computational Framework for the 3D Fully Non-Linear Dynamics of Lipid Bilayers

Author(s): *Alejandro Torres-Sánchez, Marino Arroyo, *UPC-BarcelonaTech*; Daniel Millán, *CONICET*.

In this work, we present a theoretical and computational framework for the 3D fully non-linear dynamics of lipid bilayers. Lipid bilayers are unique soft materials, operating in general in the low Reynolds limit. While their shape is predominantly dominated by curvature elasticity as in a solid shell, their in-plane behavior is that of a largely inextensible viscous fluid. This mechanical duality provides structural stability and adaptability, allowing membranes to build relatively stable structures that can nevertheless undergo dynamic shape transformations. The equilibrium behavior of lipid bilayers can be understood to a large extent with the classical bending model of Helfrich. For that reason, modeling and simulation of lipid bilayers have mainly focused on exercising Helfrich model to investigate equilibrium configurations of lipid bilayers. Beyond the Helfrich model, more general models are required to describe the dynamic transformations that bilayers undergo, which should capture the interfacial dissipative mechanisms that dominate at sub-cellular scales. Seifert and Langer developed a continuum model explicitly accounting for the bilayer architecture and capturing the major energetic driving forces and dissipative drag forces involved in the dynamics of lipid membranes. However, this model was proposed for small deviations of the geometry from a planar state and derived through a procedure based on the interfacial stress tensor, which is difficult to generalize. Here, we systematically derive a nonlinear SL theory for the dynamics of bilayer membranes in 3D. The cornerstone in this theory is Onsager's variational principle, which provides a unified framework for the dissipative dynamics of soft-matter systems. In addition to the multi-physics and geometric aspects of the theory, the three-dimensional simulation of lipid bilayers requires unconventional numerical methods since the resulting equations (1) involve higher order derivatives of the parametrization, (2) lead to a mixed system of elliptic and hyperbolic partial differential equations and (3) are stiff and difficult to integrate in time. Here, we propose a discretization based on subdivision surfaces. Regarding time integration, we show that the functional being minimized in Onsager's principle can be time-discretized, yielding variational integrators that inherit qualitative features of the time- continuous system, in particular the existence of a Lyapunov function and therefore a notion of nonlinear stability.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Near Field Equation for an Elastic Half-Space from the View Point of the Far-Field Properties of Green's Function

Author(s): *Terumi Touhei, *Tokyo University of Science*; Taizo Maruyama, *Maruyama*.

The near-field equation (Fata and Guzina, 2004) has been used for the identification of locations of scattering objects in an elastic half-space. The accuracy of the identification of scattering objects is affected by the location and number of sources and observation grids set at the free surface (Touhei et al., 2015). To investigate the accuracy, the directionality of wave propagation of Green's function is important. The far field pattern of Green's function has advantages in that it expresses the directionality of wave propagation. Nevertheless, the construction of the far-field operator for an elastic half-space is not very easy due to complex interactions of P and S waves at the free surface. Namely, the decomposition of the wavefield into P and S waves in a half-space is not self-evident. In view of the above facts, the asymptotic form of Green's function for an elastic half-space is derived and introduced into the near-field equation. The asymptotic form of Green's function is derived from the application of the steepest descent path method. The far field properties of Green's function as a result of its asymptotic form are examined based on numerical calculations. According to the numerical results, there is a region of embedded point sources, where the amplitudes of the P and S waves are prominent compared to S-P and Rayleigh waves at the free surface. In the case that scattering objects are in that region, the near-field operator is found to be well approximated by the asymptotic form of the Green's function, which decays in 1/R, where R is the distance between the source and the field point. The region is not very far from the free surface. For example, the region begins to appear around the depth of twice of the S wavelength. According to numerical results together with the mathematical structures of the near-field operator expressed by the asymptotic form of Green's function, the accuracy of the identification is discussed. Reference Fata and Guzina: Inverse Problems 20, pp. 713-736, 2004. Touhei et al.,: IJSS, 72, pp. 26-37, 2015.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Uncertainty Quantification in Multi-Scale Simulations of Coronary Artery Bypass Grafts Using Multi-Resolution Expansion

Author(s): *Justin Tran, Abhay Ramachandra, Alison Marsden, *Stanford University*; Daniele Schiavazzi, *University of Notre Dame*; Andrew Kahn, *University of California, San Diego*.

Computational simulations of coronary flow can provide non-invasive information on hemodynamics that can aid in surgical planning and research on disease progression. In this study, patient-specific geometries of coronary artery bypass grafts are constructed from CT images and finite element flow simulations are carried out using the open source software SimVascular. The results from these simulations have been previously used to report significant differences in mechanical stimuli in arterial and venous grafts in coronary bypass patients, which could possibly explain the relatively high failure rate of venous grafts [1]. The outputs of these simulations depend on a set of clinically-derived inputs that define the boundary conditions. The values of these inputs, however, are not known precisely due to limitations in measurement precision and population variability. These input uncertainties lead to uncertainty in the outputs, and these effects need to be quantified for model validation and clinical adoption. The aim of this study is to assign relative confidence on the computed hemodynamic indices hypothesized to correlate with graft failure considering two main sources of uncertainty: uncertainty in the lumped parameter boundary conditions at the inlets and outlets and uncertainty in the material properties of the vessel wall needed for deformable wall simulations. The uncertainty in the lumped parameter boundary conditions is modeled through a solution of an inverse problem. Parameter sets which produce results consistent with patient-specific data and their uncertainty, are sampled with a Bayesian parameter estimation framework. The uncertainty in the material properties of the graft vessel wall are modeled using random field theory. The variance in the material properties are assigned according to the literature, and their random distribution in space is modeled through a Karhunen-Loeve expansion which decouples the spatial and stochastic dependence of the random field. We use a generalized multi-resolution chaos approach proposed in [2] to propagate the uncertainty. The advantages of this approach lie in its ability to support inputs sampled from arbitrary joint distributions and its built-in adaptivity allowing for efficient approximations of stochastic responses characterized by sharp gradients. The main contributions to this study include quantifying relative confidence in computations of mechanical stimuli in coronary bypass grafts, and considering the combined effect of uncertainties in lumped parameter boundary conditions and wall material properties in hemodynamic simulations. References: [1] Ramachandra, A. et al., Journal of Cardiocascular Translational Research, 9.4:279-290, 2016. [2] Schiavazzi, D et al., Computer Methods in Applied Mechanics and Engineering, 314:196-221, 2017.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Calculation of T-Stress for Cracks in Two-Dimensional Anisotropic Elastic Media by Boundary Integral Equation Method

Author(s): *Han Tran, *Vietnamese-German University*.

A numerical procedure is proposed to compute the T-stress for two-dimensional cracks in general anisotropic elastic media. T-stress is determined from the sum of crack-face displacements which are computed via an integral equation of the boundary data. To smooth out the data in order to perform accurately numerical differentiation, the sum of crack-face displacement is established in a weak-form integral equation in which the integration domain is simply the crack-tip element. This weak-form integral equation is then solved numerically using standard Galerkin approximation to obtain the nodal values of the sum of crack-face displacements. The procedure is incorporated in a weakly-singular symmetric Galerkin boundary element method (SGBEM) in which all integral equations for the traction and displacement on the boundary of the domain and on the crack faces include (at most) weakly-singular kernels. To examine the accuracy and efficiency of the developed method, various numerical examples for cracks in infinite and finite domains are treated and it is shown that highly accurate results are obtained using relatively coarse meshes.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Compatible Meshfree Discretization for Dense Electrophoretic Suspension Flows

Author(s): *Nathaniel Trask, Pavel Bochev, Mauro Perego, *Sandia National Laboratories*.

Particle methods provide a flexible framework for generating boundary conforming discretizations of problems with complex deforming boundaries. Unfortunately, high-order accuracy and stability has remained elusive for these discretizations, as the lack of a mesh prevents the application of the discrete exterior calculus machinery that has been fundamental for obtaining physics compatible discretizations for mesh-based methods. We present several new compatible meshless discretizations using the generalized moving least squares framework that are able to obtain stability, scalability and accuracy competitive with their mesh-based counterparts. As an example of the types of multiphysics problems this approach allows, we consider applications in electrophoretic flows which requires the tight coupling of the steady Stokes equations for fluid flow, Poisson-Boltzmann equations for electrokinetic effects, and 6-DOF solvers for particle kinetics. We show that for each component of this problem, our discretizations are able to obtain fourth order accuracy and O(N) scaling while maintaining many unique properties which are typically only observed for compatible mesh-based methods.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Dislocation Cores from First Principles: Ni and Ni3Al for Superalloys

Author(s): *Dallas Trinkle, Anne Marie Tan, *Univ. Illinois, Urbana-Champai*.

Mechanical behavior, specifically plastic deformation at low and high temperatures in metal alloys is governed by the motion of dislocations. Dislocations in crystalline materials were hypothesized nearly eighty years ago, and their experimental and theoretical study has provided powerful tools for modern materials engineering. While the long-range elastic field of a dislocation is known and straight-forward to compute, many of the strongest effects of dislocations occur in the "core"--the center of the dislocation--where elasticity breaks down, and new chemical bonding environments can often make even empirical potential descriptions suspect. Hence, there is much effort to use the accuracy of modern density-functional theory to study dislocation cores accurately, as well as their interaction with other defects, such as solutes and boundaries. While there are a variety of possible coupling or "multiscale" techniques available, I will focus on flexible boundary conditions, which use the lattice Green's function to couple electronic structure to an infinite harmonic bulk; this approach greatly simplifies many "hand-shaking" problems, and generally provides a computationally efficient approach. This methodology has explained solid-solution softening in molybdenum (explaining a 50-year-old mystery of metallurgy), dislocation cores in aluminum and titanium, and provided a wide range of mechanical behavior predictions for magnesium alloys. For the case of nickel-based superalloys, we use density functional theory with flexible boundary conditions to compute the dislocation core structures for a 1/2<110> Ni screw dislocation and a <110> Ni3Al screw superdislocation. This also showcases our new method for computing the lattice Green function that accounts for the topology change due to a dislocation and larger partial splitting. These dislocation core structures are a first step to studying anomalous yield stress or creep mechanisms in Ni3Al from first-principles.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Structural Dynamic Analysis of an Optimized Flapping Wing Micro Air Vehicle

Author(s): *Van Tien Truong, *National University of Singapo*; Quoc Viet Nguyen , *National University of Singapore*; Marco Debiasi, *National University of Singapore* ; Heow Pueh Lee, *National University of Singapore* .

Flapping Micro aerial vehicles (FMAVs) possess many desirable characteristics such as small size, low weight, difficult to detect, highly maneuverable, and some can hover, and can be used for many applications such as surveillance, reconnaissance, search and rescue. The vibrations of the flapping wing mechanism play a significant ingredient to the stability and control of the flapping wing micro air vehicles. In a previous study, we have elaborated the structural optimization of the gearbox in a FWMAV. The topology of the spur gear and motor holder is difference from the original ones and FE analysis results has shown to meet the requirements of the mass reduction and stiffness increment. This present study is a continuation of efforts to better understand the structural performance of the optimized and original mechanism. The optimized parts were fabricated and assembled to the system. The force measurements on the optimized and original FWMAV were conducted. The natural frequency, mode shapes and deformation of gearbox components were adequately characterized by the finite element simulation. The deformation and vibration were experimentally carried out using a sensor displacement. The numerical and experimental results show that the structural performance of the optimized design has been improved greatly in comparison with original design and therefore its vibration characteristics for better fatigue life, stability and safe operation at higher flapping frequencies could be enhanced.

14th U.S. National Congress on Computational Mechanics
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Title: Crack Path Prediction in Fiber-Reinforced Composites via a Peridynamic-FEM Approach

Author(s): Srujan Rokkam, *Quang Truong, *Advanced Cooling Technologies*; Max Gunzburger, *Florida State University*; Kishan Goel, *Naval Air Systems Command*.

Peridynamics (PD) theory provides a means to investigate crack propagation behavior in solids, without the need for re-meshing the domain or other special treatments necessitated by conventional FEM approaches. As such, it has been increasing applied for modeling failure in different applications. In this work, we investigate crack propagation behavior in fiber-reinforced composite structures using a Peridynamics approach that builds on finite element method (FEM) solution kernels. The PD bonds representative of the composite are modeled as truss elements which takes into account the corresponding fiber/matrix micromechanics in definition of its constitutive behavior. The PD-FEM framework is implemented using a commercial FEA package using custom defined application programming interface (API). Subsequently, we employ it to investigate crack propagation behavior in 3D composite structures subject to various types of loading conditions. Crack propagation simulations were performed on 3-D composites with unidirectional composite at different fiber orientations and multidirectional composite (woven, multi-ply). The developed framework is able to predict crack propagation behavior based on applied loading conditions and nature of pre-existing defects. A comparison between simulated results and available literature data is also undertaken. This work was funded by NAVY SBIR Phase I program, Contract No. N68335-16-C-0301, awarded to Advanced Cooling Technologies, Inc.

14th U.S. National Congress on Computational Mechanics
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Title: A Stabilized, Symmetric Nitsche Method for Spatially Localized Plasticity

Author(s): *Timothy Truster, *University of Tennessee*.

A heterogeneous interface method is developed for combining primal displacement and mixed displacement-pressure formulations across nonconforming finite element meshes to treat volume-preserving plastic flow [1-2]. When the zone of inelastic response is localized within a larger domain, significant computational savings can be achieved by confining the mixed formulation solely to the localized region. The method's distinguishing feature is that the coupling terms for joining dissimilar element types are derived from a time-discrete free energy functional, which is based on a Lagrange multiplier formulation of the interface constraints. Incorporating residual-based stabilizing terms at the interface enables the condensation of the multiplier field, leading to a symmetric Nitsche formulation in which the interface operators respect the differing character of the governing equations in each region. The adjoint flux naturally emerges from applying the variational derivative to the Galerkin least-squares terms in the potential functional. Numerical studies are conducted for both fully discontinuous approximations and isolated discrete interfaces in order to highlight the generality of the method. Emphasis is placed upon quadratic displacement linear pressure quadrilateral elements. Optimal convergence rates are attained by the fully discontinuous approximation with respect to an exact solution, and the heterogeneous interface method achieved comparable results on coarser meshes as those obtained from applying the mixed formulation throughout the domain. References [1] T. Truster, A. Masud, Primal interface formulation for coupling multiple PDEs: A consistent derivation via the Variational Multiscale method, Computer Methods in Applied Mechanics and Engineering, 2014; 268:194-224. [2] Truster T.J., A stabilized, symmetric Nitsche method for spatially localized plasticity, Computational Mechanics, 2016; 57:75-103.

14th U.S. National Congress on Computational Mechanics
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Title: Multifrequency Interferometric Imaging with Intensity-Only Measurements

Author(s): *Chrysoula Tsogka, *University of Crete*; Miguel Moscoso, *Universidad Carlos III De Madrid*; Alexei Novikov, *Penn State University*; George Papanicoloau, *Stanford University*.

We consider here the problem of coherent imaging using intensity-only measurements. The main challenge in intensity-only imaging is recovering phase information that is not directly available in the data, but is essential for coherent image reconstruction. Imaging without phases arises in many applications such as crystallography, ptychography and optics where images are formed from the spectral intensities. The earliest and most widely used methods for imaging with intensity-only measurements are alternating projection algorithms. The basic idea is to project the iterates on the intensity data sequentially in both the real and the Fourier spaces. Although these algorithms are very efficient for reconstructing the missing phases in the data, and performance is often good in practice, they do not always converge to the true, missing phases. This is especially so if strong constrains or prior information about the object to be imaged, such as spatial support and non-negativity, are not reliably available. Rather than using phase retrieval methods, we propose a different approach in which well-designed illumination strategies exploit the spatial and frequency diversity inherent in the problem. These illumination strategies allow for the recovery of interferometric data that contain relative phase information which is all that is needed to reconstruct a so-called holographic image. There is no need for phase reconstruction in this approach. Moreover, we show that this methodology leads to holographic images that suffer no loss of resolution compared with those that use full phase information. This is so when the media through which the probing signals propagate are assumed to be homogeneous. We also consider inhomogeneous media where wavefront distortions can arise. In such media the incoherence in the recovered interferometric data can be reduced by restricting them to small spatial and frequency offsets. Using an efficient implementation of this restriction process we obtain holographic images with a somewhat reduced resolution compared to the homogeneous medium case. The robustness of our approach will be explored with numerical simulations carried out in an optical (digital) microscopy imaging regime.

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14th U.S. National Congress on Computational Mechanics
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Title: An Optimization Method for Additive-Manufactured Dental Implants

Author(s): Shih-Shun Chien, *Nien-Ti Tsou, *National Chiao Tung University*; Chang-Wei Huang, *Chung Yuan Christian University*.

The geometries of healing chamber in dental implants affect the biological healing pattern. Recently, additive-manufacturing technique opens the possibility of the shape design of the healing chamber. In addition, the shape design should not be limited by the traditional parametric design method. In this study, an evolutionary method to optimize the shape of healing chamber in additive-manufactured dental implants for better osseointegration is proposed. It adopts the modified bone remodeling algorithm [1] and is implemented by finite element software ANSYS. The concept of the proposed method is based on “survival of the fittest”. The disused bone elements located in the healing chambers, which are expected to be less likely to survive, will be replaced by implant elements. Similarly, the implant elements adjacent to the bone elements which attempt to grow, will be replaced by bone elements. The procedure will be taken iteratively, and only 1% of the elements in the healing chambers are replaced at each iteration in order to avoid the dramatic change of the geometries of the implant. The objective of the procedure is to maximize the fraction of the healthy surrounding bone and bone-implant-contact area. It allows an automatic formation of a complicated configuration of the healing chamber. The method is applied to a ITI dental implant for posterior maxillary bones with a vertical load of 100 N. Based on the calculation, the optimized implant gives the volume fraction of the healthy surrounding bone about 13% compared with it of the commercial ITI implant. The shape of the healing chamber shares several features in common with the bone geometries due to the remodeling process observed in experiments. The current optimization method is sufficiently general to extend to other types of implants and loading conditions. [1] Jiyean Kwon, 2010. Simulation Model of Trabecular Bone Remodeling Considering Effects of Osteocyte Apoptosis and Targeted Remodeling. Journal of Biomechanical Science and Engineering, 539–551.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Nonlocal Updated Lagrangian Particle Hydrodynamics Method and Simulation of Underwater Explosion

Author(s): *Qingsong Tu, Yumeng Hu, Shaofan Li, *CEE, UC Berkeley*.

The numerical simulation of underwater explosion has been a long standing challenging problem for many decades, due to the high pressure and shock wave propagation created by the explosion. In this work, we have developed a novel nonlocal updated Lagrangian Particle hydrodynamics (ULPH) method, and we have applied to simulate underwater bubble motion and underwater explosion. First, a meshfree non-local differential operator approach is developed in current configuration. Rigorous mathematics proofs are given to show that both the spatial meshfree gradient operator and the spatial meshfree divergent operator are convergent. Secondly, the nonlocal meshfree differential operators are applied to the Navier-Stocks equations, and we established a set of consistent discrete particle hydrodynamics based on the mass, momentum, and energy conservation laws by using the non-local differential operators. Third, a ULPH/SPH coupling algorithm is developed to couple the fluid particles with explosive particles, and Fourth the equation of state of explosive, the constitutive equation of nearly incompressible viscous fluid, and free surface effects are all carefully studied and implemented for the simulation of underwater explosion. Several benchmark problems of different boundary conditions have been tested, and the simulation results are validated by both the experimental data and other numerical results in the literature. The proposed model is capable of analyzing the complex variables such as energy change and exploding velocity; all these quantities are measured to monitor convergence toward a reference solution. The results of this new method agree very well with benchmark results and experimental data; Also, a detailed comparison of the new method with SPH method shows that the proposed method has distinct computational advantages over SPH. In conclusion, the proposed ULPH method is robust and stable enough to accurately simulate the dynamic phenomena of rising bubbles in different conditions, which can give a reference for engineering applications.

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Title: Fluid-Structure Interaction Of Dacron Aortic Prostheses Conveying Pulsatile Flow

Author(s): Marco Amabili, *Eleonora Tubaldi, Michael p. Païdoussis, *McGill University*.

Dacron represents the standard material for large-diameter vascular grafts used in various circumstances of vascular maladies requiring replacements of components of the cardiovascular system, such as vessel patches for aneurysms. The main disadvantages of such grafts are reduced compliance and reduced tissue incorporation. The compliance mismatch between arteries and grafts can cause flow disruption, increase the risk of thrombosis and it is known to reduce graft patency. Wide knowledge about the distinctly different mechanical properties of the Dacron implants with respect to the native aorta is available in literature while very little is known about the dynamic behavior of these prostheses. This study addresses for the first time the dynamic response to pulsatile physiological blood flow and pressure of a woven Dacron graft currently used in thoracic aortic replacements. Artificial blood vessels can be modeled as thin-walled shells conveying pulsating flow. The prosthesis is modeled as a circular cylindrical shell described by means of the nonlinear Novozhilov shell theory. The material considered is orthotropic and the boundary conditions are flexible (distributed axial and rotational springs) to simulate the connection with the host artery. The blood flow is modeled as a Newtonian pulsatile flow, and pulsatile viscous effects are taken into account. Coupled fluid-structure Lagrange equations for a non-material volume with wave propagation in case of pulsatile flow are applied. Physiological waveforms of blood pressure and flow velocity are approximated with the first eight harmonics of the corresponding Fourier series. Time responses of the radial displacement of the artificial vessel during exercise are compared to the ones at rest. Differences in the frequency content contributions are presented and discussed. Frequency-response curves in the physiological range show the geometrically nonlinear vibration response to pulsatile flow. During exercise (i.e. high pulsatile flow velocity and high heart rate) the bifurcation diagrams present several superharmonic resonance peaks. The effect of different values of modal damping on the dynamic behavior of the prosthesis is investigated. In the limit case of low modal damping values, the prosthesis can lose stability with deformation in the cross-section by ovalization modes of the shell (shell-like buckling). In this deformed condition, high stress localized regions appear in the inner wall and flow separation or turbulence can develop eventually causing the failure of the prosthesis. Preliminary experimental results of modal damping values estimated by experimental modal analysis tests of a woven Dacron graft are also presented.

14th U.S. National Congress on Computational Mechanics
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Title: Goals of the Exascale Additive Manufacturing Project (ExaAM)

Author(s): *John Turner, Balasubramaniam Radhakrishnan, *Oak Ridge National Laboratory*; James Belak, Nathan Barton, Jean-Luc Fattebert, Neil Hodge, Wayne King, *Lawrence Livermore National Laboratory*; Sudarsanam Babu, *University of Tennessee, Knoxville*; Curt Bronkhorst, Christopher Newman, *Los Alamos National Laboratory*; Neil Carlson, ; Lyle Levine, *National Institute of Standards and Technology*.

Additive manufacturing (AM), or 3D printing, of metals is transforming the fabrication of parts by reducing the weight of final parts, reducing waste (and hence energy) in the manufacturing process, and dramatically expanding the design space, allowing optimization of shape and topology. However, there remain challenges in qualification of AM parts due to the unique physical phenomena inherent in AM processes. Although the physical processes involved in AM are similar to those of welding, a field with a wealth of experimental, modeling, simulation, and characterization research over the past decades, the failure rate for new AM parts is often as high as 80%. While modeling approaches and simulation tools for welding and similar processes are quite mature, and have been calibrated to the point that they are approaching predictive capability, they are inadequate for AM processes. We believe this is because the process-structure-property-performance relationship is traditionally treated in an uncoupled manner, relying on tabular databases that are unable to adequately capture the rapid dynamics and non-equilibrium nature of AM processes. The Exascale Additive Manufacturing Project (ExaAM) has been initiated as an integrated collaboration between U.S. Dept. of Energy laboratories as part of the Exascale Computing Project (ECP). ECP is a broad program that includes hardware, system software, system acquisition, and science application development. ExaAM is one of the applications selected for the development and implementation of models that would not be possible on more moderate computational systems. With the prospect of Exascale computing resources in mind, one of the goals of ExaAM is to remove the limitations noted above by coupling high-fidelity sub-grid simulations within continuum process simulations to determine microstructure, properties, and hence performance using local conditions. We will briefly describe the overall goals and elements of ECP as well as the technical approach being taken in ExaAM, and how it can ultimately enable a priori specification of local structure, properties, and performance of even the most complex AM parts.

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Title: Simulations of Fracture of Amorphous Solids by Multiscale Cohesive Zone Model

Author(s): *Shingo Urata, *Asahi Glass Co., Ltd.*; Shaofan Li, *UC-Berkeley*.

A Multiscale Cohesive Zone Model (MCZM) has been developed to simulate fracture and crack propagations in solids by combining cohesive zone model with an atomistically enriched constitutive relation in the framework of finite element method. The method has been successfully applied to simulate fracture of crystalline materials in both 2D and 3D. In this study, we extend the method with combining the Cauchy-Born rule and the Parrinello-Rahman molecular dynamics (MD) method in order to apply the MCZM to simulate fracture in amorphous materials. The new algorithm utilizes a representative cell (r-cell) composed of multiple atoms and their configurations are associated with material deformation, then the first Piola-Kirchhoff stress is evaluated based on the local interatomic interaction. We have validated the computational formulation and algorithm by comparing the simulation results with that of MD simulations for amorphous silicon and Lennard-Jones binary glass. The amorphous r-cells were constructed by NPT MD simulations of quenching from high temperature. Material responses of cubic specimen, in which the r-cell was embedded, were simulated in cases of both uniaxial and shear deformations, and we found our method can reasonably reproduce stress-strain curve obtained by MD simulations even though relatively small number of atoms are utilized in the r-cell. Moreover, we have successfully simulated crack growth in the two amorphous materials by using the multiscale cohesive zone modeling, and it was found that the extended MCZM can capture both brittle and ductile fractures in amorphous materials. The computational physics model is further extended to study the fracture in polycrystalline material by modeling non-crystalline structure in grain boundary as a type of amorphous material. We have shown that under the common loading condition the fracture path of a single-notched polycrystalline thin specimen is always intergranular, and it compares well with the result with large size MD simulations.

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Title: Divergence Free Virtual Elements

Author(s): Lourenço Beirão da Veiga, *Giuseppe Vacca, *University of Milano Bicocca*; Carlo Lovadina, *University of Milano*.

The Virtual Element Method is a generalization of the classical Finite Element Method to arbitrary element-geometry. In the first part of the talk we present a new family of Virtual Elements for the Stokes problem on polygonal meshes. By a proper choice of the Virtual space of velocities and the associated degrees of freedom, we can guarantee that the final discrete velocity is pointwise divergence-free, and not only in a relaxed (projected) sense, as it happens for more standard elements. Moreover, we show that the discrete problem is immediately equivalent to a reduced problem with fewer degrees of freedom, thus yielding a very efficient scheme. The focus of the second part of the talk is on developing a Virtual Element Method for Darcy and Brinkman equations. We use introduce a slightly different Virtual Element space having two fundamental properties: the L2-projection onto the space of polynomials of degree k (being k the order of the method) is exactly computable on the basis of the degrees of freedom, and the associated discrete kernel is still pointwise divergence-free. The resulting numerical scheme for the Darcy problem has optimal order of convergence and H1 conforming velocity solution. In particular we obtain a Virtual Element scheme that is accurate for both Darcy and Stokes equations. Then we can apply the same approach to develop a stable virtual element method for Brinkman equations (that is combination of Stokes and Darcy equations). We provide a rigorous error analysis of the method and several numerical tests, including a comparison with a different Virtual Element choice.

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Title: Wave Characteristics of 1D and 2D State-Based Peridynamics in Comparisons with Nonlocal General Gradient Theory

Author(s): *Senthilkumar Vaiyapuri, *CSIR Fourth Paradigm Institute*.

Recently developed nonlocal general gradient theory for 1D bar has been investigated. This model consists of two different characteristics length scales. The Peridynamics[1] model consists of one length scale parameter. The bond-based and state-based bar models with 1D and 2D Peridynamics are compared for dispersion, phase velocity and group velocity with nonlocal general gradient model. Further different nonlocal weight functions are used in the present wave characteristics studies. Reference 1. Z.P. Bažant, W.Luo, V.T. Chau and M.A. Bessa, "Wave Dispersion and Basic Concepts of Peridynamics Compared to Classical Nonlocal Damage Models", J. Appl. Mech, 83 (11), 111004-16, 2016, doi: 10.1115/1.4034319.

14th U.S. National Congress on Computational Mechanics
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Title: Wind-Structure Interaction as an Aid to Establish the Design Wind Pressures of Tensile Membrane Structures

Author(s): *J. Gerardo Valdés-Vázquez, A. David García-Soto, Alejandro Hernández-Martínez, L. Francisco Gay-Alanís, *University of Guanajuato*.

Some decades ago, membrane structures were used to span large facilities at economical costs. Nowadays, a wider scope of applications of this structures is noticeable, such as solar shading, protection against rain, bus stations, market places, etc. This is a consequence of the advent of new textile fabric materials. Modern tensile fabric structures are known to have low self-weight and an optimal stress distribution, since they work only in tension because of an initial prestress, usually induced mechanically or pneumatically. However, only a few basic national design codes for specific types of tensile fabric structures are available in some countries, despite of a considerable amount of scientific knowledge of their structural behavior. The main drawback for designing a tensile fabric structure is the correct distributions of wind pressures and its highly non-linear behavior. Since wind loads for tensile membrane structures can be found using a wind-tunnel analysis, in this work a computational fluid-structure interaction scheme is used as an alternative method. To take into account the warp and weft behavior of tensile membrane structures, first an orthotropic non-linear finite element analysis of prestressed membrane structures is used. Then, wind simulation is performed with finite elements by solving the Navier-Stokes equations, via the fractional step method with the orthogonal sub-scales stabilization procedure. Finally, a fluid-structure interaction is coupled with a staggered partitioned scheme. Since the computational work of the fluid-structure interaction scheme has been previously validated, an application for two different mechanically prestressed tensile fabric structures is study and, as a result, wind pressure patterns are recommended to complete the design process of the studied tensile fabric structures without the need of wind tunnel test.

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Title: Modeling Competing Hydraulic Fracture Propagation Using Generalized/Extended Finite Element Method

Author(s): *Dakshina Valiveti, *ExxonMobil Upstream Research C*; Fushen Liu, Peter Gordon, *ExxonMobil Research and Engineering Company*.

Successful stimulation of low permeability reservoirs requires the creation of closely spaced fractures that provide conduits for fluid production. This is accomplished by pumping fluid at high rates in closely grouped perforation clusters, in the hopes that multiple fractures will simultaneously propagate into the formation. In many cases, however, production log data has suggested that only a fraction of perforation clusters appear to contribute to overall production. It is suspected that the mechanical interaction of incipient fractures attempting to propagate simultaneously is a primary reason that only a subset preferentially form. In this talk, we present a framework for numerical simulation of hydraulic fractures using the Generalized Finite Element method (GFEM) with two popular fracture model descriptions: Linear Elastic Fracture Mechanics (LEFM) and the Cohesive Zone Model (CZM). Both models simulate fluid driven fracture propagation in poro-elastic/elastic media. The discontinuities across the fracture face in displacement and pore-pressure field are handled using special enrichment functions within GFEM framework. Fluid flow inside the fracture is governed by the lubrication equation and is solved using a local pressure field across fracture surface. In the LEFM approach, fracture tip stress intensity factors and fracture toughness govern the fracture propagation [1], whereas in the CZM approach the cohesive law drives the fracture [2]. We will present numerical examples of competing fracture growth using each model, examining the effects of fracture spacing and driving force on the resultant fracture growth patterns. References: [1]. Valiveti, D. M., Meier, H. A., Liu, F., & Gordon, P. A., Numerical Simulation of 3D Hydraulic Fractures in Poro-Elastic Rocks. Proceedings of 13th International Society for Rock Mechanics (ISRM) Congress of Rock Mechanics, Montreal, Canada, 2015 [2] F. Liu, P.A. Gordon, H.A. Meier, D.M. Valiveti. A stabilized extended finite element framework for hydraulic fracturing simulations. International journal for numerical and analytical methods in Geomechanics, 2016.

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Title: A PDE-Based Overhang Constraint in Topology Optimization for Additive Manufacturing

Author(s): *Emiel van de Ven, *Netherlands Aerospace Centre, TU Delft*; Matthijs Langelaar, Can Ayas, Fred van Keulen, *TU Delft*; Robert Maas, *Netherlands Aerospace Centre*.

The complex nature of designs resulting from topology optimization often prevents direct implementation of optimized designs. Consequently, post-processing of the optimized design is often required to make it manufacturable. This is not only labour intensive, but also reduces the optimality. Therefore, additive manufacturing has gained an increasing amount of attention within the topology optimization community since it allows for much larger form freedom compared to conventional production methods such as milling or casting. Additive manufacturing builds a product layer upon layer. As long as there is a sufficient connection between the layers, almost any design can be built: complexity comes with no extra cost. However, additive manufacturing also has some process limitations. There is for example a minimum feature size, a minimum hole size, and the overhang limitation, which is the focus of this study. Because each layer needs a sufficient support from the previous layer, there is a limitation on the orientation of free surfaces. This is often measured by the minimum angle a surface can make with the base plate: the minimum overhang angle. By incorporating a minimum overhang angle into the topology optimization process, resulting designs can be readily printed without any alterations or the addition of support structures. This can save machine, material and labour costs. Only few overhang constraints have been presented, most notably by Gaynor and Guest (2016) and Langelaar (2016). However, these constraints are either highly non-linear or mesh dependent. In this study, a constraint is formulated in the continuous domain, making it mesh independent. It is based on the Hamilton-Jacobi-Bellman PDE, which can be solved efficiently with the use of front propagation methods. The additive manufacturing process is approximated by a propagating front. Overhanging regions can subsequently be identified by inspection of the arrival times of the propagation. With the use of adjoint sensitivities, the constraint can be used in the optimization process to suppress overhang. Numerical examples will be presented on unstructured meshes with the focus on 3D cases. Gaynor, A.T., & Guest, J.K. (2016). Topology optimization considering overhang constraints: Eliminating sacrificial support material in additive manufacturing through design. Structural and Multidisciplinary Optimization, 54(5), 1157-1172 Langelaar, M. (2016). An additive manufacturing filter for topology optimization of print-ready designs. Structural and Multidisciplinary Optimization, 1-13.

14th U.S. National Congress on Computational Mechanics
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Title: Thermodynamic Consistency and Stable Schemes for Quasi-Incompressible Navier-Stokes-Cahn-Hilliard Models

Author(s): Gorkem Simsek, Mahnaz Shokrpour Roudbari, E. Harald van Brummelen, *Technische Univ. Eindhoven*; *Kris van der Zee, *Univ. of NOTTINGHAM*.

We introduce a thermodynamically-consistent quasi-incompressible diffuse-interface Navier-Stokes Cahn-Hilliard model for two-phase-flow of incompressible fluids with different densities. Its derivation is based on mixture theory by invoking the second law of thermodynamics and the Coleman-Noll procedure. In addition, we propose a linear and energy-dissipative time-integration scheme for the derived model. Such a scheme is nontrivial, because it has to suitably deal with all nonlinear terms in the model, and appears to be the first linear method that satisfies a discrete energy law for quasi-incompressible two-phase flows. Numerical experiments verify the suitability of the scheme for high density ratios and for large time step sizes by considering the coalescence and break-up dynamics of droplets including pinching due to gravity. Reference: G. Simsek, K.G. van der Zee, M. Shokrpour Roudbari, and E.H. van Brummelen, “Linear and Energy Dissipative Scheme for Two-Phase-Flows of Quasi-Incompressible Navier-Stokes Cahn-Hilliard Models”, ArXiv:1603.06475, (2016)

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Title: Multi-Scale Modelling of Structure Evolution in Tungsten under Irradiation and Heat Loads

Author(s): *Hans van Dommelen, Awital Mannheim, Marc Geers, *Eindhoven University of Tech.*.

Nuclear fusion is potentially an important future source of energy. Critical for the development of a fusion reactor that is economically viable is the lifetime of the so-called divertor. This is the component through which energy in the form of heat is extracted from the fusion reactor and tungsten is a commonly chosen material for it. In addition to the heat load, this device is also subjected to large neutron and plasma loads. In particular, the neutron load will lead to the accumulation of lattice damage in the polycrystalline structure of the material. The combination of a continuous source of lattice damage and a high temperature in some locations leads to an evolution of the microstructure in the form of recovery, grain growth and possibly recrystallization. At the same time, these processes affect the thermo-mechanical properties of the material and thereby the functionality of the device. In this work, a multi-scale model for the irradiation-induced lattice damage, the resulting microstructural evolution processes, and the thermomechanical consequences is developed. Thereby, this approach bridges length scales ranging from the level of lattice point defects (in the form of vacancies and interstitials) to the polycrystalline microstructure and to the scale of a tungsten monoblock. The development of neutron-induced lattice damage is described using a Cluster Dynamics model [e.g., 1] that accounts for primary damage sources due to irradiation and the recombination of defects to vacancy and interstitial clusters of various sizes, as well as the development into a dislocation network. The lattice defect free energy serves as a driving force for microstructure evolution in a mean field recrystallization model with multiple homogeneous equivalent media, as proposed in [2] for dynamic recrystallization. This modelling approach accounts for the various competing processes in the material, depending on the temperature. The evolving microstructural characteristics in the form of grain size distribution and lattice defects govern the thermomechanical properties in a macroscopic numerical analysis of a tungsten monoblock under heat loading. References [1] T. Jourdan, Journ. of Nucl. Mat., 467, 286-301 (2015). [2] P. Bernard, et al., Mat. Sci. Eng. A, 528, 7357-7367 (2011).

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Title: Quantification and Modelling Geometrical Variability in Composite Fibre Reinforcement Data

Author(s): *Dirk Vandepitte, Ilya Straumit, Stepan V. Lomov, *KU Leuven*; Andy Vanaerschot, *Brussels Airlines*.

Non-determinism requires much attention in the certification procedure of complicated structural components. Composite materials are gaining much interest because of their high performance, especially for transportation applications. However, the multitude of design, material and process parameters add to the complexity of the analysis, and procedures for certification and quality assurance are demanding. Uncertainty and scatter on critical material parameters need to be quantified in close relation to the application and also to the production process which is used, with a particular focus on the geometrical characteristics of the fibre reinforcement architecture. In this paper, the authors develop a general 3 step approach to quantify variability on geometrical tow parameters (x, y and z co-ordinates of tow centroid position, tow area, tow aspect ratio and orientation), based on experiments with extensive data analysis. The first step is the collection of experimental data and the subsequent statistical analysis. Two length scales are considered, one on the level of the representative volume element using μCT and the other on the scale of multiple unit cells. The former set gives precise positional and cross-sectional data on the meso-level. Average trends, standard deviation and correlation lengths are identified. The second step is the stochastic multi-scale modelling, including the definition of systematic and handling trends from the experimental data, the generation of zero-mean deviations correlated along and between neighbouring tow paths. Cross-correlations are taken into account, a cross-correlated series expansion is used, based on a Karhunen-Loève decomposition, as proposed by Vorechovsk■ [1]. In the third and final step, WiseTex models are generated. WiseTex [2] is a pre-processor for the generation of virtual 3D models of a wide range of textile composite architectures. The pre-processor prepares for the generation of finite element models for the mechanical analysis of composite structures. The statistics of the virtual models which are generated match all statistical characteristics of the hardware samples, both in short range and in long range. The procedure is applied to a carbon fibre reinforcement system with a complicated multi-layer architecture which is designed for a thermal protection system in a spacecraft for entry, descent and landing of science and exploration class payload missions. Statistics of the full set of the generated samples match the statistics of the experimental data set. References: [1] M. Vorechovský, D. Novák, Correlation control in small-sample Monte Carlo type simulations 1: A simulated annealing approach, Probabilistic Engineering Mechanics, 24(3):452-462, 2009. [2] http://www.mtm.kuleuven.be/Onderzoek/Composites/software/wisetex, 2015.

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Title: System-Level Validation of the Warrior Injury Assessment Manikin Finite Element Model

Author(s): *Nicholas Vavalle, *Johns Hopkins APL*; Matthew Shanaman, Christian Lomicka, Parth Patel, *Johns Hopkins Applied Physics Lab*.

The Warrior Injury Assessment Manikin (WIAMan) Anthropomorphic Test Device (ATD) will serve as a state of the art Soldier surrogate for Under Body Blast (UBB) testing. A finite element model of the ATD, developed in conjunction with the manikin, accelerated the design process and reduced risk for the implementation phase of the ATD. Further, the model will serve as a long-term complement to the physical ATD for live-fire testing and evaluation. The model can be used to predict failure and confirm physical ATD survivability in extreme loading scenarios. The ability of the model to accurately predict physical ATD responses was characterized against several validation cases. The objective of this work is to present the level of validation of the WIAMan FEM in system-level simulations. The WIAMan FEM was developed and validated using a hierarchical approach. Polymer materials in the ATD were experimentally characterized and material models were optimized to these data. Component models were developed and validated individually and then incorporated into the full system-level model. The focus of the current work is the whole body validation. The model has been simulated in three loading conditions to which the physical technology demonstrator ATD was subjected. The Vertically Accelerated Load Transfer System at the Johns Hopkins Applied Physics Lab applied unique inputs to the floor and seat with the ATD in various personal protective equipment configurations. The model validation was quantified using the cross correlation (CC) score of correlation and analysis (CORA) which compares the model to experimental outputs with a rating from zero to one. The corridor portion of CORA was omitted because the variance in the physical ATD response was low. The typical simulation time for the WIAMan FEM is approximately two days for a 100 ms simulation on 60 processors. As an indication of model stability and verification, the hourglass energy ratio to internal energy is less than 5% in all three simulations. In total, 33 signals were evaluated for each of the three signals including accelerations, rotations, forces, and moments. The mean CORA CC scores for the three simulations were 0.71, 0.71, and 0.74. In addition to a quantitatively validated model, model processing tools have been developed to enhance the user community productivity. A tool that utilizes the LS-PrePost ATD positioning capabilities to position the model into various postures has been developed. This can allow a user to place the model into alternate postures and vehicle configurations. On the post-processing end, a standalone executable has been developed to output selected signals from the model that match the physical ATD channels with various filtering and display options. These capabilities allow a user to leverage model information much faster than without such tools. DISTRIBUTION STATEMENT A - APPROVED FOR PUBLIC RELEASE; DISTRIBUTION IS UNLIMITED

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Title: A Workflow for Thermal-Mechanical Modeling of Additive Manufacturing

Author(s): *Michael Veilleux, Michael Stender, Lauren Beghini, Joshua Sugar, Samuel Subia, *Sandia National Laboratories*.

The focus of this presentation is a multi-physics workflow for modeling additive manufacturing (AM) of metals that represents temporally and spatially varying thermal profiles and residual stresses resulting from material deposition and cooling processes. The AM process of interest is Laser Engineered Net Shaping (LENS®), a Directed Energy Deposition (DED) technology wherein metal powder is sprayed into a scanning, focused laser beam to create a moving melt pool. A Lagrangian finite element analysis methodology is chosen to model the underlying phenomena: laser-induced heating; material activation; thermal radiation, convection, and conduction; liquid-to-solid transition; re-melting; evolution of temperature-dependent material properties and bonds (e.g. to the substrate); and, thermally driven deformation and residual stress accumulation. The movement of the laser beam is modeled in discrete steps; the phenomena are modeled iteratively and all history dependence is mapped forward over each iteration. This workflow elucidates the process parameters that affect residual stresses and produce properties of interest in additively manufactured parts. *Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: A Bayesian Approach to Model Calibration, Selection and Surrogate Modeling: Application to Traumatic Brain Injury

Author(s): *Kumar Vemaganti, Emily Kang, *University of Cincinnati*; Sandeep Madireddy, *Argonne National Laboratory*.

Computational models of the head and brain are extensively used to study traumatic brain injuries (TBI). Simulations of TBI are complex and computationally challenging because of (a) the large uncertainty in the material testing data and the resulting uncertainty in the constitutive model parameters, (b) high strain rates and the short time scales of the impact loading, and (c) the complex geometry of the human brain model. We describe a Bayesian framework for parameter estimation and constitutive model selection based on the parallel nested Monte Carlo sampling algorithm MULTINEST. Four different factors are used to reliably choose a parsimonious model from the candidate set of models. These are the qualitative fit of the model to the experimental data, evidence values, maximum likelihood values, and the landscape of the likelihood function. This approach provides a robust and efficient alternative to Markov chain Monte Carlo methods to sample from multi-modal distributions and to efficiently calculate the evidence integral. Brain tissue in general has a non-linear visco-hyperelastic constitutive response. In this study, the long-term viscoelasticity, the short-term viscoelasticity, and hyperelasticity contributions to the mechanical response of the brain tissue are modeled separately. The distributions of the corresponding parameters are obtained using the nested sampling-based Bayesian framework. This constitutive model is then implemented into the finite element code LS-DYNA. Traumatic brain injury caused by impact loading from a vehicle crash is simulated using the SIMon finite element model of the human head. A maximum principal strain-based injury criterion is used to assess the severity of the brain injury. The uncertainty in the material model parameters is non-intrusively propagated to the injury criterion using a Bayesian Gaussian process surrogate of the finite element model to avoid computationally expensive simulations. This enables us to calculate the probability that an injury tolerance is reached for a given impact loading. This probabilistic method can be used to further simulate injuries and calculate various injury criteria with high fidelity.

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Title: Homogenization Based on Realization-Dependent Hashin-Shtrikman Functionals of Piecewise Polynomial Trial Polarization Fields

Author(s): *Nicolas Venkovic, Lori Graham-Brady, *Johns Hopkins University*.

Our objective is to draw a better understanding of the relation between the mechanical response of polycrystals and their morphology. To do so, we investigate the dependence of the Hashin-Shtrikman (HS) functional on the morphology of random microstructures, realization-by-realization. Upon successive Taylor expansions of the Green operator for strains, some estimates of the influence tensors that arise in the HS functionals for piecewise polynomial trial polarization fields of arbitrary orders are formulated in terms of Minkowski tensors. This approach differs from the way the HS bounds are traditionally constructed in that it does not seek to optimize the ensemble average of a random functional. Instead, an extensive characterization of the morphological anisotropy of every single realization of a random microstructure is carried over, hence allowing relaxation of any type of assumption of morphological symmetry of the medium. The accuracy of the method and its dependence on the estimates of the influence tensors is investigated for different polynomial orders of trial polarization fields in polycrystalline microstructures with different elastic material symmetries. After validation of the framework for elastic loadings of polycrystals, the possibility of applying the method to viscoplastic and elastic-viscoplastic behaviors using affine representations of the local constitutive responses is investigated.

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Title: Quadrilateral Mesh Adapation Using Approximate Convex Scaffolding

Author(s): *Chaman Singh Verma, Krishnan Suresh, *Univ of Wisconsin, Madison*.

Mesh adaptation plays a critical role in balancing computational efficiency and numerical accuracy. Three types of mesh adaptation techniques exist today, namely, mesh improvement, mesh refinement and mesh simplification, and, for each of these, several algorithms have been proposed. Current mesh adaptation algorithms yield acceptable geometric mesh quality, but provide limited control over topological quality. Many existing quadrilateral meshes exhibit non-local topological dependencies which makes their dynamic adaptation non-trivial. The non-local behaviour in such meshes is caused by non-optimal configuration of singularities (nodes which have non-ideal number of adjacent faces). Unfortunately, singularities are essential to control maximum geometric distortion in a mesh and therefore they may be necessary for a high-quality mesh. In the talk, I will show how singularities can also be used to achieve localized quadrilateral meshes (LQM). When a mesh is localized, then any modification in its topology affects only a small region of the mesh. We achieve LQM by first creating approximate convex scaffolding of a given model. This scaffolding in created once in the beginning, and thereafter frozen from further modifications. Then, in each approximate convex sub-domain, we use specific alpha-MST templates which allow all types of mesh adaptation without crossing the scaffolding. The rationale behind choosing approximate convex sub-domains instead of strict convex sub-domains is that unnecessary singularities may appear otherwise. By using approximate convex domains, we effectively reduce the number of singularities. Using several examples, we demonstrate how specific configuration of singularities in each convex sub-meshes could (1) improve both geometric and topological qualities of a quadrilateral mesh, (2) provide efficient data interpolation in adaptive applications, and (3) avoid element inversion during large mesh deformation.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Optimal Runge-Kutta Schemes for Pseudo Time-Stepping with High-Order Methods

Author(s): *Brian Vermeire, *Concordia University*; Niki Loppi, Peter Vincent, *Imperial College London*.

In this presentation we will provide optimal Runge-Kutta (RK) schemes for solving the pseudo-time problem introduced via the Artificial Compressibility Method (ACM) paired with high-order spatial discretizations. We will provide RK schemes that are optimal in this context for the Discontinuous Galerkin (DG) and Spectral Difference (SD) methods, each recovered via the Flux Reconstruction (FR) approach. These RK schemes are optimal in the sense that they allow the largest possible pseudo time-step to be taken per RK stage for linear advection. We find that each optimal RK scheme depends on the number of RK stages, the polynomial degree of the spatial discretization, and the chosen FR correction function. We will provide new schemes using up to seven RK stages and with spatial discretizations up to polynomial degree k=8. Results show that these schemes can be at least 80% faster than the classical fourth-order RK scheme (RK4) when applied to linear advection problems. This represents a significant speedup, and in practice is achieved via trivial code modification. We will then demonstrate that these schemes can be implemented using the ACM in the open-source solver PyFR, and used to solve a variety of unsteady incompressible flow problems. Finally, we will provide a computational cost comparison between these new optimal RK schemes and conventional schemes that are currently used in practice with the ACM for unsteady incompressible turbulent flows.

14th U.S. National Congress on Computational Mechanics
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Title: Patterning and Morphogenesis of Cortical Folding

Author(s): *Sarah Verner, Krishna Garikipati, *The University of Michigan*; Shiva Rudraraju, *The University of Wisconsin*.

While recent computations have demonstrated symmetric cortical folding, it is notable that most brains (including those of humans) demonstrate small variations from perfect symmetry. These asymmetric foldings are critical for the formation of sulci and gyri which position important brain centers. We seek to study the physical processes that lead to asymmetric folding. While understanding the mechanics and mathematics underlying this complex phenomenon is motivating from a theoretical perspective, it also has the potential to enrich our comprehension of human brain development. This knowledge could eventually have far-reaching implications in our diagnosis, prevention and treatment of several brain development anomalies including polymicrogyria (over abundance of smaller brain folds), pachygyria (reduced number of folds that are unusually shallow) and lissencephaly (absence of folds), as well as many others. It has been established that the sulcification and gyrification of the brain result from elastic buckling, and post buckling deformation. These result from circumferential stress induced by inhomogeneous local growth. However, given what is known about neurological development, it seems obvious that neuronal birth near the ventricles, followed by migration into the cortex and accumulation there must play a role in the location of sucli and gyri. This also suggests an origin for asymmetric folding. Another hypothesis is the influence of boundary conditions on the ventral side of the brain. The present work aims to explore both these approaches as well as provide the framework for future data-driven modeling of brain folding.

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Title: Computational Modeling of Hydrogel-Based Tissue Engineering: En Route to Personalized Regenerative Medicine

Author(s): *Franck Vernerey, Shankar Sridhar, Stephanie Bryant, *University of Colorado-Boulder*.

Despite tremendous advances in the field of tissue engineering, a number of obstacles remain that hinder its successful translation to the clinic. A particular challenge relates to the choice of a biomaterial that can guide the growth process and simultaneously provide a temporary mechanical support for developing tissue. Synthetic-based hydrogels are particularly promising as they can be engineered with precision while mimicking the natural cell environment. A major challenge however is to understand and identify how hydrogel structure and functionality enable cell-mediated tissue synthesis, transport and deposition while providing a mechanical support that can resist physiological loads at the early stage of implementation. A solution to this problem has been to balance tissue growth and hydrogel degradation. However, identifying this balance is difficult due to the complexity of coupling diffusion, deposition, and degradation mechanisms. Very little is known about the complex behavior of these mechanisms, emphasizing the need for a rigorous mathematical approach that can assist and guide experimental advances and switch regenerative medicine from a phenomenological to a predictive, physics-based discipline. This presentation will discuss a model for interstitial growth based on mixture theory, which can capture the coupling between cell-mediated hydrogel degradation (i.e., hydrogels containing enzyme-sensitive crosslinks) and synthesis/transport of extracellular matrix (ECM) molecules. Taking cartilage tissue engineering as an example, the model investigates the role of bulk and localized degradation on ECM diffusion and its impact on two important outcomes: the extent of ECM transport (and deposition) and the successful transition, in terms of mechanical integrity, between the hydrogel and the neo-tissue. Numerical results based on finite element analysis suggest that non-uniform, localized hydrogel degradation and a heterogeneous cell distribution are key elements for this successful transition and ultimately to achieve tissue growth. Specifically, we find that cell-mediated, localized degradation and the presence of well-connected and dense cell clusters create optimum conditions needed for neo-tissue growth while maintaining structural integrity. Experimental observations using cartilage cells encapsulated in a hydrolytically degradable hydrogel are compared with model predictions to show the potential of the proposed model.

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Title: Multigrid Methods for Crack Propagation and Contact

Author(s): Rolf Krause, Alena Kopanicakova, Patrick Zulian, *Cyrill von Planta, *USI Lugano*.

We present and discuss multigrid methods, which are especially designed to solve contact problems as well as spatial problems arising in crack propagation. Although multigrid methods are by now well established tools for the solution of large scale problems in mechanics, their application to problems involving complex domains or contact and internal interfaces is far from trivial, since the multi-level hierarchy has to be designed carefully in order to preserve the optimal complexity of the method. In particular when dealing with natural geometries, setting up the nested multilevel hierarchy for optimal efficiency can become tedious. Here, we overcome this problem by employing discrete L^2-projections to facilitate the Galerkin assembly of the multilevel hierarchy and obtain semi-geometric multigrid methods, which we further adapt to their specific problem class, i.e. crack propagation and contact. As a first example, we consider crack propagation modelled by means of a phase field approach. By introducing a damage parameter, this approach avoids the explicit representation of discontinuities and possible remeshing. The downside is a higher complexity in terms of number of unknowns and of the arising discrete systems, as a coupled non-linear system for displacements and damage parameter has to be solved. We show that our semi-geometric multigrid shows excellent performance on the arising linearized systems. As a second example, we consider contact problems for which we employ a solution dependent choice of the multilevel hierarchy. The resulting semigeometric and monotone multigrid methods have the advantage that they resolve the contact conditions locally and do not need an inner/outer iteration scheme. We simulate laboratory experiments with granite specimens collected from the Grimsel test-site in Switzerland. The meshes are obtained using high resolution photogrammetry scans for which it is virtually impossible to construct nested hierarchies of meshes, as would be needed by geometric multigrid methods. We will present numerical examples for both problem classes and show that the semi-geometric multigrid concept leads to highly efficient solution methods. Moreover, some comparisons with algebraic multigrid methods will be presented.

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Title: Dendrite Fragmentation and the Columnar-to-Equiaxed Transition During Solidification

Author(s): T. Cool, E.B. Gulsoy, *P.W. Voorhees, *Northwestern University*.

A particularly important issue with the additive manufacturing of metallic parts is the grain structure of the resulting part. Depending on the processing parameters, columnar or equiaxed grain growth is present, while in other cases there is a transition from columnar to equiaxed grains (CET). The importance of the CET lies in the clear connection between the properties of the solidified ingots and the grain structure. For example, ingots with elongated grains can have much different creep behavior than those with equiaxed grains. Moreover, if the conditions under which the CET occurs are well understood, a properly placed CET can be used to tailor the properties of the part, as well as the spatial distribution of the intergranular eutectic. The presence of undercooled liquid in front of the growing columnar dendrites implies that nucleation of solid is possible. Given the solidification rates and degrees of undercooling, nucleation usually occurs heterogeneously. For example, the dendritic mush itself can be the source of the nucleants via fragmentation of existing columnar dendrites. These fragments are then transported by convection ahead of the tips of the columnar dendrites into the undercooled liquid region, and then form equiaxed grains. The mechanism by which dendrites fragment remains controversial. The fragmentation process has been studied using 3D reconstructions of a solid-liquid mush in the absence of gravitationally induced sedimentation in both Pb-Sn and Al-Si alloys. The results of these experiments will be shown. We have also used experimentally measured microstructures as initial conditions in phase field calculations. These phase field calculations are then used to follow the evolution of the microstructure, thus providing important insights into the processes governing the dendrite fragmentation process, and the source of heterogeneities that can be responsible for the dendrite-to-equiaxed transition.

14th U.S. National Congress on Computational Mechanics
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Title: Multi-Physics Coupling Challenges and Approaches for Modeling Thermally Activated Batteries

Author(s): *Tyler Voskuilen, John Hewson, Harry Moffat, Scott Roberts, *Sandia National Laboratories*.

The activation process for LiSi/FeS2 thermally activated batteries is a complex coupled process involving energetic material burn, heat transport, phase change, capillary-driven two-phase porous flow, ion transport, electrochemical reactions, and mechanical deformation [1]. There are both strong and weak couplings between many of these physical processes that can influence the prediction of key battery metrics such as the time to electrochemical activation, the operating voltage under load, and the battery lifetime. Prior models of the activation process have included only subsets of these processes with various coupling strategies [2]. In this work, we explore the relationship between the degree and method of coupling for different physical processes and the predicted response and computational cost. Of particular emphasis in this work is the effect of including the mechanical deformation and the degree to which it is coupled to the porous flow and electrochemical processes. We compare the computational cost and variability in predictions obtained using a monolithic coupling and a segregated coupling with varying degrees of model dependence between the different physical processes. We discuss metrics for defining which model dependencies to include or omit with a focus on characteristic time scales of coupling for transient problems. A key question for any multi-physics coupled problem is where reduced order models can be used without compromising a simulation's prediction accuracy. Based on the coupling study and time scale metrics, we also evaluate the effect of a proposed reduced order model to allow us to remove some of the more computationally costly physical models from our simulations. 1. S. Roberts, K. Long, J. Clausen, M. Martinez, E. Piekos, A. Grillet, Towards a Coupled Multiphysics Model of Molten Salt Battery Mechanics, Proceedings of the 46th Power Sources Conference, 2014 2. T. Voskuilen, J. Hewson, H. Moffat, S. Roberts, Multi-Physics, Multi-Plateau Reaction Model for LiSi/FeS2 Batteries, Proceedings of the 47th Power Sources Conference, 2016

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Title: Multi-Scale Simulation of Rubber Fracture Using Space-Time FEM and Non-Ordinary State-Based Peridynamics

Author(s): *Shogo Wada, Dong Qian, *University of Texas at Dallas*.

Rubbery materials are widely used in the industry, e.g., tire, engine mount, seismic isolation rubber, mechanical sealing, etc. Prediction of the failure of rubber is essential to ensure the safety and integrity of many applications. However, simulation-based prediction of rubber failure remains a significant challenge due to the extremely long temporal scale and large number of load cycles, which are generally beyond the capability of conventional FEM-based tools. In addition, capturing failure initiation and progression in rubber requires robust computational representations beyond mesh-based discretization. In this presentation, we propose a multiscale method that couples the space-time Finite Element Method with peridynamics for the simulation of dynamic fracture problems of rubber. In the temporal domain, space-time FEM based on the time-discontinuous Galerkin method [1, 2] is proposed. In the spatial domain, enriched FEM approximation is first introduced to represent global deformation and the crack path. A fine scale region is further prescribed around the crack tip and non-ordinary state-based peridynamics [3] is applied for simulating crack initiation and propagation. The crack path in the coarse domain is updated based on peridynamics and the interfacial boundary condition is established to couple between peridynamics and FEM. Robustness of this coupled method is demonstrated through examples of rubber fracture prediction. Acknowledgement: S. Wada would like to thank the Bridgestone Co. for a fellowship of the graduate study. References [1] T. J. R. Hughes and G. M. Hulbert, “Space-time finite element methods for elastodynamics: formulation and error estimates,” Comput. Methods Appl. Mech. Eng., vol. 66, pp. 339–363, 1988. [2] S. Bhamare, T. Eason, S. Spottswood, S. R. Mannava, V. K. Vasudevan, and D. Qian, “A multi-temporal scale approach to high cycle fatigue simulation,” Comput. Mech., vol. 53, no. 2, pp. 387–400, 2014. [3] T. L. Warren, S. A. Silling, A. Askari, O. Weckner, M. A. Epton, and J. Xu, “A non-ordinary state-based peridynamic method to model solid material deformation and fracture,” Int. J. Solids Struct., vol. 46, no. 5, pp. 1186–1195, 2009.

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Title: Evaluation of Elastic-Plastic Fracture Simulation for Compact Tension Specimen Subjected to Low Cycle Fatigue

Author(s): *Yoshitaka Wada, *Kindai University*.

Crack growth under elastic-plastic fracture is an important issue of the structural integrity, because seismic waves cause low cycle fatigue in the engineering structure. Many researchers have conducted experiments and numerical analyses, however obvious and general criteria cannot be found until now. In order to develop a three-dimensional fracture criterion, the fully automated and state-of-the-art FE crack growth simulation should be realized. In the numerical simulation system, there are three important processes namely, generation of the model with crack, stable and accurate FE analysis, and post-processing for fracture evaluation. Crack growth simulation requires each process to be stable and connected to each other in one system. On the other hand, experiments should be conducted to determine material properties such as cyclic stress strain curve, crack tip opening displacement, J-integral, etc. In particular, determination of parameters for appropriate cyclic stress strain curve is very important to actual evaluation of seismic loading. We have developed an automatic mesh generation system for precise crack surfaces with thumbnail crack front and shear lip crack surface using a second order tetrahedral element. The present work shows the result of generation phase analysis of a compact tension specimen in comparison with several constitutive equations, because cyclic stress-strain curve was very sensitive for load and load line displacement in the past work. The work shows comparisons between experimental results and numerical simulation results. We discuss the appropriateness of a constitutive equation to reproduce the relationship between load and load point displacement in the low cycle fatigue.

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Title: Multi-Scale Solidification Simulations of Additive Manufacturing Process in Metals

Author(s): *Gregory Wagner, Stephen Lin, Wing Kam Liu, *Northwestern University*.

The material microstructure in parts produced through additive manufacturing is known to be very sensitive to the parameters governing the process. For example, in powder-bed or powder deposition processes, the porosity and the grain size and shape are affected by the laser power, path, and scan speed. Many of these effects can be traced to the complex thermal history at locations in the part as material is repeatedly melted, cooled, and reheated through multiple build layers and laser passes. In this work we model the development of metal microstructure during solidification by simulating the process at two different scales: the part scale, giving temperature fields throughout the part during the entire build, and the microscale, allowing microstructure development and growth to be simulated at select locations. At the part scale, we use an efficient finite element solution of the heat equations, including an effective heat capacity model informed by a database computed in ThermoCalc to capture the thermodynamics of solidification for a specific material. At the microscale, we use a cellular automata/finite element (CAFE) model to simulate the growth and interaction of individual grains. The two scales are coupled through the space- and time-varying temperature field. Through this approach we study the effects of various process parameters and toolpath designs on the resulting grain structures of the finished part.

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Title: Stability Analysis of Metals Capturing Brittle and Ductile Fracture through a Phase Field Method and Shear Band Localization

Author(s): Miguel Arriaga, *Haim Waisman, *Columbia University*.

Dynamic fracture of metals may be brittle or ductile depending on factors such as material properties, loading rate and specimen geometry. At high strain rates, a thermo plastic instability known as shear banding may occur, which typically precedes fracture. A thermodynamically consistent model which accounts for both shear banding and dynamic fracture and can thus capture both failure bodes at intermediate strain rates, is proposed. The model consists of an elastic-viscoplastic material with strain hardening, strain rate hardening, and thermal softening. Fracture is modeled with the phase field method, for which a novel modification is presented here to account for the creation of fracture surfaces by inelastic work. In this presentation I will focus on model derivation, implementation and stability analysis to determine the onset of shear or fracture localization, based on a linear perturbation analysis. Numerical results will be presented to illustrate the predictive capabilities of the unified model and the stability criterion obtained. References [1] McAuliffe C. and Waisman H., 2015, “A unified model for metal failure capturing shear banding and fracture,” International Journal of Plasticity, 65:131-151. [2] McAuliffe C. and Waisman H., 2016, “A coupled phase field shear band model for Ductile-Brittle transition in notched plate impacts,” Computer Methods in Applied Mechanics and Engineering, 305:173–195. [2] Arriaga M., McAuliffe C. and Waisman H., 2015, “Onset of shear band localization by a local generalized eigenvalue analysis,” Computer Methods in Applied Mechanics and Engineering, 289:179-208.

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Title: Multiphysics Design Optimization Using an Adjoint Sensitivity Approach

Author(s): *Stuart Walker, *Altair*.

Optimal design methods involving the coupling of fluid and structural solutions are a topic of active research; particularly for aerospace applications. The paper presents a coupled fluid and structure approach to topology optimization using two commercial finite element solutions; AcuSolve and OptiStruct. A gradient based method is used to minimize the compliance of a structure subject to thermal loading. The optimal material distribution to minimize compliance is computed using the Solid-Isotropic Material with Penalty (SIMP) method available in OptiStruct. A volume fraction constraint is imposed in order to iteratively reduce the parts mass. Draw constraints are used to ensure manufacturability. The thermal loading is computed iteratively using a computational fluid dynamics (CFD) solution from AcuSolve. The optimization produces an innovative design which increases the heat rejection rate of the part while reducing the mass.

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Title: Advanced Higher Order Methods and Modified Inverse Analyis for Improved Photoacoustic Biomedical Image Reconstruction

Author(s): Svenja Schoeder, Martin Kronbichler, *Wolfgang A. Wall, *TU Munich*.

Photoacoustic imaging is a comparably new imaging method based on the photoacoustic effect and its application ranges from imaging of small animals or inflammatory arthritis to breast cancer detection. The functional principle is as follows: An examination object is illuminated with a laser light flash. The laser light then propagates within the object according to its optical properties and is absorbed. Subsequently, the energy transforms via thermal expansion to ultrasound waves, which is called the photoacoustic energy conversion. The ultrasound waves are detected as acoustical signals at the object's boundary that are used as input for a reconstruction process of the material properties. In this talk we present novel computational approaches – both for the forward solution of this opto-acoustic problem as well as for the reconstruction. The novelty in the forward model lies in the acoustic part of this opto-acoustic problem. We have developed an attractive high order Hybridizable Discontinuous Galerkin (HDG) method and propose a novel new time integrator, that allows being arbitrary high order in time while maintaining the characteristic superconvergence properties of HDG. For the reconstruction step we propose an approach that, on the one hand, combines identification of the different effects in one inverse analysis sweep and, on the other hand, enables a better handling of heterogeneities. We will present the essentials of the methods, show some simple numerical examples to prove and highlight their numerical features as well as apply it to some real biomedical imaging example. References: [1] S. Schoeder, M. Kronbichler, W.A. Wall, Photoacoustic Image Reconstruction: Material Detection and Acoustical Heterogeneities. Inverse Problems, accepted 2017. [2] S. Schoeder, M. Kronbichler, W.A. Wall, Arbitrary High-Order Explicit Hybridizable Discontinuous Galerkin Methods for the Acoustic Wave Equation. submitted 2017. [3] M. Kronbichler, S. Schoeder, Müller, C., W.A. Wall, Comparison of implicit and explicit hybridizable discontinuous Galerkin methods for the acoustic wave equation. International Journal for Numerical Methods in Engineering, 106 (2016), 712-739.

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Title: Design Optimization of Mechanical Metamaterials for Vibration Control

Author(s): *Timothy Walsh, Josh Robbins, Chris Hammetter, *Sandia National Laboratories*; Wilkins Aquino, *Duke University*.

Harsh shock and vibration environments are commonly encountered in engineering applications involving dynamic loading. Acoustic/elastic metamaterials are showing significant potential as candidates for controlling wave propagation and isolating sensitive structural components. While the complex microstructures of these materials can be realized with additive manufacturing, they must be properly designed to achieve their desired properties. In this talk we will present time and frequency-domain strategies for PDE-constrained design optimization of elastic/acoustic metamaterials, focusing on multiphase composite and lattice structures as candidate materials. A frequency-domain approach is typically the desirable strategy when designing band-gap or notch filter materials, whereas a time-domain strategy may be advantageous in a transient shock environment. For the frequency-domain optimization, a Modified Error in Constitutive Equation (MECE) objective function will be compared with the least squares counterpart in terms of effectiveness for designing a material that provides a notch filter. For the time-domain, a transient optimization formulation will be presented and demonstrated on a vibration isolation problem. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed martin Corporation, for the U.S. Department

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Title: Advances in Coupled ALE-AMR for Tetrahedral Grids

Author(s): *Jacob Waltz, Jozsef Bakoski, *Los Alamos National Laboratory*.

Adaptive mesh refinement (AMR) and arbitrary Lagrangian-Eulerian (ALE) methods both have long and successful histories in computational fluid dynamics, shock hydrodynamics, and related fields. AMR methods are typically implemented in an Eulerian framework to increase mesh resolution at discontinuities, where solution accuracy is limited to first-order. ALE methods, which treat the mesh coordinates as an additional degree of freedom, are often implemented in a Lagrange-plus-remap form to maintain mesh robustness during extreme fluid distortion. ALE methods also can be used to allow mesh motion relative to the Eulerian reference frame for problems such as aeroelasticity and store separation as well as shock hydrodynamics. Despite their individual records of success, few examples of coupled ALE-AMR methods can be found in the published literature. Although such a methodology may appear to simply require that both ALE and AMR are implemented in the same code and compatible at the software level, this is a necessary but not sufficient condition. A useful analogy is coupled multi-physics simulation : different physics packages must not only be implemented in the same code but also coupled in a physically correct manner. Similarly, ALE and AMR methods must be coupled in a mathematically correct manner. This coupling is therefore the primary subject of this work. The goal of the coupled method is to use AMR to reduce numerical error in ALE simulations at reduced computational expense relative to uniform fine mesh calculations, in the same manner that AMR has been used in Eulerian simulations. We also identify deficiencies with ALE methods that AMR is able to mitigate, and discuss the unique coupling challenges. The coupled method is demonstrated using three-dimensional unstructured meshes of up to 10^7 tetrahedral cells. Speed-ups of 5-10x are observed relative to uniform fine mesh calculations.

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Title: A Reliability Analysis Method for Assessment of Concrete Barriers under Vehicle Crashes

Author(s): *Qian Wang, *Manhattan College*; Hongbing Fang, *The University of North Carolina at Charlotte*; Hanfeng Yin, *Hunan University*.

Due to the inherent randomness in various crash and impact problems, reliability analyses of these problems become more important for decision making in engineering design. In this work, a probability-based analysis method for assessing the performance of concrete median barriers under vehicle crashes was studied. The parameters of a vehicular impact, such as the impact angle and the weight of vehicle were considered as random variables. Nonlinear finite element analysis was employed to calculate velocities and accelerations of a vehicle, and other crash responses. To reduce the high computational cost of reliability analyses due to the required large number of nonlinear transient dynamic simulations, a metamodeling technique was applied. The metamodels, which were created using radial basis functions (RBFs), had no error on the sample data points. Once the metamodels were generated for the dynamic crash responses, they were used in the reliability analysis based on Monte Carlo Simulations (MCS). This proposed approach was very efficient, especially for crash and impact problems involving expensive numerical simulations and a small number of random variables. This method was demonstrated to be useful for various mathematical and practical engineering examples, based on the authors' previous research work. In this study, various crash responses including vehicle responses and occupant injury criteria based on vehicle responses were considered and reliability analyses were conducted. The failure probabilities obtained based on the RBF metamodels and MCS were found to provide useful information for design and assessment of concrete barriers.

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Title: Limitations of Multi-Scale and Multi-Physics Modeling

Author(s): *Sheldon Wang, *Midwestern State University*.

With the advent of computer software and hardware, it is now possible to study the system behaviors for large coupled systems with multiple scales and physics. However, it important to emphasize the unpredictability issues in this era of irrational exuberance partially attributed by wanton hubris [9][10][12][13]. In 1980s, many researchers have discovered the unpredictable behaviors stemmed from coupled nonlinear dynamical systems with three or more state variables. Although the governing equations are deterministic, just as predicted by Henri Poincare [6], due to the fact that the differential manifolds are very close to each other, with even an infinitesimal amount of perturbation, which is essentially unavoidable in modern computing or real world simply governed by the second law of thermodynamics, the solution in time can be completely transformed. The so-called chaotic phenomena have been reported in the past three decades from various branches in social and natural sciences [5]. Now we are clear that a positive Lyapunov exponent tends to generate chaotic behaviors [4]. In fact, even the very established genius like von Neumann could make an incorrect statement in 1950 to predict long term phenomena of meteorology with so-called sufficiently large computers. Economists and sociologists are still making similar mistakes [10][11]. Is it possible different multiscale systems are similar to each other when they are approaching the jump of phase or scale? The universal Feigenbaum number confirms such a concept [5][7]. In fact, similar power law distributions are the manifestations of the fractal dimensions in chaotic systems with many interactive factors. The evidence of rich and poor gap is a good example for the power law distribution in any unbounded complex system just like Pareto 80-20 principle [8], Max Kleiber's law on metabolic rate [7], turbulent boundary layer [1][2], Paul Paris law on crack propagation [3], and S-N curve for fatigue [3]. Keywords: Complex system modeling, Phenomenological rule, Power law, and chaos. Reference 1. Allen, M.P.; Tildesley, D.J.: Computer Simulation of Liquids. Clarendon Press, New York, NY, USA (1989). 2. Berge, P.; Pomeau, Y.; Vidal, C.: Order within Chaos - Towards a deterministic approach to turbulence. John Wiley & Sons (1984). 3. C.Bathias: There is no infinite fatigue life in metallic materials. Fatigue & Fracture of Engineering Materials & Structures, 22, 7, (1999), 559--565. 4. D. Otter, W.K.; Briels, W.J.: Free energy from molecular dynamics with multiple constraints. Molecular Physics: An International Journal at the Interface between Chemistry and Physics, 98, 12, (2000), 773--781. 5. Gleick, J.: Chaos -Making a new science. Viking (1987). 6. Hadamard, J.: The early scientific work of Henri Poincare. The Rice Institute Pamphlet, 9, 3, (1922), 111--183. 7. M. Kleiber: Body size and metabolism. Hilgardia, 6, (1932), 315--351. 8. Pareto, V.: Manual of Political Economy. Augustus M. Kelley (1971). 9. Schlick, T.: Molecular Modeling and Simulation: An Interdisciplinary Guide. Springer Verlag (2002). 10. Greenspan, A.: The Age of Turbulence. Penguin, (2008). 11. Dyson, F. (2007). Heretical thoughts about science and society. Edge: The Third Culture 12. T. Wu, S. Wang, B. Cohen, and H. Ge, "Molecular Modeling of Normal and Sickle Hemoglobins," International Journal for Multiscale Computational Engineering, 8, pp 237-244, 2010. 13. T. Wu, S. Wang, and B. Cohen "Modeling of Proteins and Their Interactions with Solvent," in Advances in Cell Mechanics. Chapter 3, pp. 55-116, Springer, ISBN 978-3-642-17589-3, 2011.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Intercalation Driven Porosity Effects in Coupled Continuum Models for the Electrical, Chemical, Thermal and Mechanical Response of Battery Electrode Materials

Author(s): *Zhenlin Wang, Jason Siegel, Krishna Garikipati, *University of Michigan*.

We present a coupled continuum formulation for the electrostatic, chemical, thermal and mechanical processes in battery materials. Our treatment applies on the macroscopic scale, at which electrodes can be modelled as porous materials made up of active particles held together by binders and perfused by the electrolyte. Starting with the description common to the field, in terms of reaction-transport partial differential equations for ions, variants of the classical Poisson equation for electrostatics, and the heat equation, we add mechanics to the problem. Our main contribution is to model the evolution of porosity as a consequence of strains induced by intercalation, thermal expansion and mechanical stresses. Recognizing the potential for large local deformations, we have settled on the finite strain framework. We have carried out a detailed computational study on the influence of the dynamically evolving porosity, via the electrostatic and reaction-transport coefficients, upon ion distribution, electrostatic potential fields, and charge-discharge cycles.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Numerical Simulations of the Richtmyer-Meshkov Instability of the “Inverse Chevron” Interface

Author(s): *Tao Wang, *Institute of Fluid PhysicsCAEP*.

The classical Richtmyer-Meshkov instability is a complex phenomenon which happens at a geometrical perturbed interface between two different fluids when a shock wave passes through the interface. The mechanism is the baroclinic vorticity production owing to the misalignment of the pressure gradient of across the shock front and the local density gradient at the perturbed interface. At the late times the Richtmyer-Meshkov instability will induce the turbulent mixing. This phenomenon is great significant in a variety of man-made applications and natural phenomena such as inertial confinement fusion (ICF), high-speed combustion and astrophysics (i.e. supernova explosions), and has gained much attention all long. In this paper, by using our in-house large-eddy simulation code MVFT (multi-viscous- flow and turbulence)[1,2], we have numerically simulated the AWE’s shock tube experiment of inverse chevron perturbation with three sets of grids and the largest amount up to 1 billion and 24 million, and studied the double interface (air/SF6/air) Richtmyer-Meshkov instability and the turbulent mixing. The inverse chevron perturbation is located at the SF6/air interface, and the incident shock wave with Mach number 1.26 moves along the direction of air/SF6/air. The calculated positions of large scale wall bubble and spike for different grid resolution has a very small difference and agree with experiment quantitatively, but statistics quantities such as turbulent kinetic energy, enstrophy, are not grid-converged. The numerical simulations also show the reflections, transmissions and refractions of shock waves at the double interface and the very subtle multi-scale spatial structures of turbulent mixing zone.

14th U.S. National Congress on Computational Mechanics
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Title: Material-Dependent Crack-Tip Enrichment Functions in XFEM for Modeling Bimaterial Interfacial Cracks

Author(s): *Yongxiang Wang, Haim Waisman, *Columbia University*.

A novel set of enrichment functions within the framework of the extended finite element method (XFEM) is proposed for linear elastic fracture analysis of interface cracks in bimaterials. The motivation for the new enrichment set stems from the revelation that the accuracy of the widely accepted 12-fold bimaterial enrichment functions significantly deteriorates with the increase in material mismatch. To this end, we propose an 8-fold material-dependent enrichment set, derived from the analytical asymptotic displacement field, that well captures the near-tip oscillating singular fields of interface cracks, including the transition to weak discontinuities of bimaterials. The performance of the proposed material-dependent enrichment functions is studied on two benchmark examples. Comparisons are made with the 12-fold bimaterial enrichment as well as the classical 4-fold homogeneous branch functions which have also been used for bimaterials. The numerical studies clearly demonstrate the superiority of the new enrichment functions, which yield the most accurate results but with less number of degrees of freedom and significantly improved conditioning than the 12-fold functions. Furthermore, material-dependent high-order enrichment set, up to the order of two, is also derived to improve the accuracy of near-tip fields, enabling a direct evaluation of the complex stress intensity factors (SIFs) of interface cracks through Irwin's crack closure integral. The proposed method is shown to work well on several benchmark examples involving straight and curved interface cracks, giving accurate SIF results.

14th U.S. National Congress on Computational Mechanics
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Title: A New Very Large Eddy Simulation of the Flow over a Cylinder at Low Re=3900

Author(s): *Shuangfeng Wang, Puxian Ding, *South China University of Tech*.

In this paper, flow over a cylinder at low Reynolds number 3900 is simulated by a new Very Large Eddy Simulation (VLES) model. The aim of the current work is to evaluate the performance of VLES model in the prediction of flow over a cylinder. A new VLES model is firstly proposed based on the BSL RANS model. A new control resolution function is obtained to clip the turbulent viscosity based on the Speziale's VLES model. The proposed VLES model can behave as RANS near the wall and as VLES away from the wall. Secondly, the model is tested by the comparison of LES, DES and experimental results. The Strouhal number, mean separation angle, mean recirculation length, mean drag, RMS of lift coefficient, mean velocity and RMS of velocity are selected as the comparative variables. The results show that the proposed VLES model give a satisfactory prediction in simulating flow over a cylinder at low Re=3900.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Improved Wall-Modeling for Large Eddy Simulation Using the FR/CPR Method

Author(s): *ZJ Wang, *University of Kansas*; Jingchang Shi, Hong Yan, *Northwestern Polytechnical University*.

High-order methods have demonstrated their potential in large eddy simulations (LES) of turbulent flows with relatively low Reynolds numbers. The cost becomes a serious limiting factor for high Reynolds number problems. A promising approach to reduce the cost of these simulations is to model the near wall flow. In this paper, an improved wall modeling approach for the high-order FR/CPR method is developed, and demonstrated for high Reynolds flow problems.

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14th U.S. National Congress on Computational Mechanics
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Title: Primal-Dual Weak Galerkin Finite Element Methods for PDEs

Author(s): *Junping Wang, *National Science Foundation*; Chunmei Wang, *Texas State University*.

This talk will introduce a primal-dual finite element method for variational problems where the trial and test spaces are different. The essential idea behind the primal-dual method is to formulate the original problem as a constrained minimization problem. The corresponding Euler-Lagrange formulation then involves the primal (original) equation and its dual with homogeneous data. The two equations are linked together by using properly-defined stabilizers commonly used in weak Galerkin finite element methods. The primal-dual method will be discussed for three type of model problems: (1) second order elliptic equation in nondivergence form, (2) steady-state linear convection equations, and (3) elliptic Cauchy problems. Weak Galerkin (WG) is a finite element method for PDEs where the differential operators (e.g., gradient, divergence, curl, Laplacian etc.) in the weak forms are approximated by discrete generalized distributions. The WG discretization procedure often involves the solution of inexpensive problems defined locally on each element. The solution from the local problems can be regarded as a reconstruction of the corresponding differential operators. The fundamental difference between the weak Galerkin finite element method and other existing methods is the use of weak functions and weak derivatives (i.e., locally reconstructed differential operators) in the design of numerical schemes based on existing weak forms for the underlying PDEs. Weak Galerkin is a natural extension of the classical Galerkin finite element method with advantages in many aspects. The goal of this talk is to demonstrate some of these advantages in numerical PDEs. The talk will start with the second order elliptic equation, for which WG shall be applied and explained in detail. In particular, the concept of weak gradient will be introduced and discussed for its role in the design of weak Galerkin finite element schemes. The speaker will then introduce a general notion of weak differential operators, such as weak Hessian, weak divergence, and weak curl etc. These weak differential operators shall serve as building blocks for WG finite element methods for other class of partial differential equations, such as the Stokes equation, the biharmonic equation, the Maxwell equations in electron magnetics theory, div-curl systems, and PDEs in non-divergence form. The speaker will then discuss the primal-dual technique for the three model problems. The talk should be accessible to graduate students with adequate training in computational mathematics.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Nesting Sub-Domain Gradient Smoothing Integration Scheme for Meshfree Methods

Author(s): *Dongdong Wang, Junchao Wu, *Xiamen University, China*.

An efficient nesting sub-domain gradient smoothing integration scheme is proposed for Galerkin meshfree methods with particular reference to the quadratic exactness. Firstly, a rational measure is devised to evaluate the error for the gradient smoothing integration of stiffness matrix in the quadratic meshfree formulation. Subsequently, a nesting sub-domain gradient smoothing integration scheme is successively built upon the smoothed gradients of meshfree shape functions defined on two-level nesting triangular sub-domains, where each integration cell consists of four equal area nesting sub-domains. According to the current error measure, it turns out that an optimal combination of the two-level gradient smoothing integrations is capable of completely eliminating the integration error of stiffness matrix. Meanwhile, the integration of force terms consistent with the stiffness integration is presented in order to ensure exact quadratic solutions within the Galerkin formulation. Finally, both efficiency and accuracy of the proposed nesting sub-domain gradient smoothing integration scheme are demonstrated through a set of numerical examples. Acknowledgements: The support of this work by the National Natural Science Foundation of China (11472233, 11222221) is gratefully acknowledged.

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14th U.S. National Congress on Computational Mechanics
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Title: Mixed Bernstein-Bézier Discretizations of Trimmed CAD Surfaces for Isogeometric Analysis

Author(s): *Wei Wang, Xiaoxiao Du, Gang Zhao, *Beihang University*; Howie Fang, *The University of North Carolina at Charlotte*.

Isogeometric analysis on complex geometries built with multiple trimming NURBS patches has been always regarded as a tough process for practitioners due to the problems like the imposition of Dirichlet boundary conditions, integration of trimmed elements, coupling of non-conforming patches and the convergence of the approximations. Nevertheless, trimming and jointing operations are commonly used in the NURBS-based geometric modeling because they provide great flexibility for representation of the surfaces with complicated topologies and offer an intuitive work style for CAD designers. Motivated by the mesh generation in the classical FEA processes, in this paper, trimmed NURBS surfaces are converted into several geometrically exact meshes consisting of tensor-product (rectangular) Bézier patches and triangular Bézier patches for isogeometric analysis. It provides an advisable method to analyze topology-complex geometries with isogeometric approach. The elements on a trimmed NURBS surface are classified into three types: non-trimmed elements, trimmed elements and invalid elements accordingto the definition of the trimming curves and NURBS surfaces. Rectangular Bézier patches can be exactly extracted from the non-trimmed elements by using knot insertion algorithms and triangular Bézier patches are converted from the trimmed elements. It is straightforward for us to generate conforming meshes along the interfaces between different NURBS patches. Meanwhile, h-refinement and p-refinement can be easily achieved on the converted meshes. The trimming boundaries are replaced by the boundaries of mixed Bernstein-Bézier patches which means we can directly impose Dirichlet boundary conditions on the trimming boundaries. In addition, Gaussian quadrature rules are employed to compute the integration over rectangular and triangular Bézier patches. Classical finite element codes can be introduced to analyze mixed Bernstein-Bézier patches with a minor modification on the shape functions subroutine where Lagrange basis functions are substituted by Bernstein basis functions. Several numerical examples including 2D elasticity, static bending and free vibration of plates and shells are investigated to verify the robustness, accuracy and convergence of the proposed method.

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Title: Spectrum Slicing Using Chebyshev Polynomials

Author(s): *Xin Wang, *UCCS*; Michael Lee, Jaroslaw Knap, *U.S. Army Research Laboratory*.

Subspace iteration approaches (Zhou et al., 2006, Motamarri et al. 2014, etc.) to density functional theory (DFT) are gaining popularity in the real-space DFT community. After reducing the many degrees of freedom from the real-space grid to a smaller subspace that is of the order of the number of electrons in the system using subspace projections, if one is interested in the orbitals of the systems, a full eigensolve is required for the remaining degrees of freedom. For system sizes beyond 10,000 electrons, this eigensolve would contribute significantly to the computational cost of the DFT calculation. Spectrum slicing is good way of dividing the work of finding the lowest subset of eigenvectors in parallel manner. Schofield et al. (2012) had demonstrated the effectiveness of using Chebyshev-Jackson polynomials for spectrum slicing and Motamarri et al. (2017) had used Chebyshev polynomials to remove the core-electrons orbitals from the subspace. We will demonstrate an alternative use of the Chebyshev polynomials to perform spectrum slicing that is comparable in effectiveness as above mentioned approaches.

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Title: An Accelerated Diffusive Molecular Dynamics Method for the Simulation of Nonlinear Mass Transport in Nanomaterials

Author(s): Xingsheng Sun, *Kevin Wang, *Virginia Polytechnic Institute and State University, United States*; Pilar Ariza, *Universidad de Sevilla, Spain*; Michael Ortiz, *California Institute of Technology, United States*.

Diffusive Molecular Dynamics (DMD) is a class of recently developed computational models for the simulation of long-term diffusive mass transport at atomistic length scale. Compared to previous atomistic models (e.g., transition state theory based accelerated molecular dynamics), DMD allows the use of larger time step sizes, but has a higher computational complexity at each time step due to the need to solve a nonlinear optimization problem at every time step. This talk presents two numerical methods to accelerate DMD simulations. First, we show that when a multibody potential function (e.g., embedded atom method (EAM)) is employed, the cost of DMD is dominated by the calculation of the expectation of the potential function (and its derivatives), which is a high-dimensional random variable. To reduce the cost, we explore both first- and second-order mean field approximations. Specifically, we show that the first-order approximation, which can be viewed as using Jensen's inequality as an equality, can reduce the cost by one to two orders of magnitude, but may introduce relatively large error in the solution. We show that adding an approximate second-order correction term can significantly reduce the error without much increase in computational cost. Second, we show that DMD can be significantly accelerated using subcycling time-integrators, because the cost of integrating the empirical diffusion equation is much lower than that of the optimization solver. To assess the numerical approximation methods, and to demonstrate the capability of DMD, we present several large-scale simulations of hydrogen diffusion in metal nanomaterials (specifically, single-crystalline palladium nanoparticles). In particular, we show that DMD is capable of capturing the slow phase boundary propagation and the small lattice misorientation in the process of phase transformation, which are in good agreement with recent experimental studies.

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Title: Locally Conservative Essentially Non-Oscillatory Solution Transfer for Multiphysics Coupling

Author(s): Xiangmin Jiao, *Xuebin Wang, Qiao Chen, *Stony Brook University*.

Solution transfer is an important problem in multiphysics applications, especially for code coupling in a partitioned approach, where each physics component solves on its own mesh and may use different discretization methods. In these simulations, the meshes are in general non-matching, and the solution data must be exchanged frequently between different meshes. There are many competing requirements for solution transfer, including accuracy, conservation, monotonicity preserving, efficiency, robustness, etc. These requirements make the problem decidedly challenging. The consistent interpolation methods can achieve reasonable accuracy but it is not conservative and may lead to overshoot or undershoot. The conservative schemes, such as the common-refinement based method [2], are accurate and conservative, but they are more complicated to implement, more expensive to compute, and more difficult to achieve high-order accuracy and robustness. In this work, we propose a general framework for solution transfer, which can overcome the limitations of the previous methods. Our framework is based on two key components: a weighted-least-squares-based essentially non-oscillatory (WLS-ENO) scheme [3] and a Petrov-Galerkin formulation [1]. The WLS-ENO scheme allows higher-order accurate reconstructions of the solution in smooth regions, while automatically resorting to locally conservative, lower order schemes near discontinuities or large gradients to avoid over- shoots or undershoots. Unlike the common-refinement based method [2], which is a finite element method and requires solving a global linear system, the new approach is analogous to a hybrid finite-difference and finite-volume method unified under the Petrov-Galerkin formulation with adaptive test functions and requires solving smaller, more localized linear systems. Therefore, the new method is more efficient and scalable, and it can adapt more easily to complex functions and geometric domains. Our method applies to structured meshes, unstructured meshes, and point clouds, and it supports both node-centered and cell-centered data in finite difference, finite element, and finite volume methods. We report preliminary results in 1-D, 2-D and 3-D. References [1] R. Conley, T.J. Delaney, and X. Jiao, Overcoming Element Quality Dependence of Finite Elements with Adaptive Extended Stencil FEM (AES-FEM), International Journal for Numerical Methods in Engineering, Vol. 108, pp. 1054–1085, 2016. [2] X. Jiao and M. T. Heath. Common-refinement-based data transfer between nonmatching meshes in multiphysics simulations. International Journal for Numerical Methods in Engineering. Vol 61, pages 2402-2427. December 2004 [3] H. Liu and X. Jiao. WLS-ENO: Weighted-Least-Squares Based Essentially Non-Oscillatory Schemes for Finite Volume Methods on Unstructured Meshes. Journal of Computational Physics. Vol. 314, pp. 749- 773, 2016.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Coarse-Grained Model for Cell Nuclear Pore Complex and Nanoparticles Interaction

Author(s): *Xianqiao Wang, Liuyang Zhang, *University of Georgia*.

Understanding and controlling the selective nanoparticle transport through the nuclear pore complex is critical to the development of nanomedicine applications. The transport happens about milliseconds and the length scale of hundreds of nanometers; however, the fundamental transport mechanism remains elusive due to lack of suitable experimental and/or computational tools. By taking into account the elastic structure of nucleus envelope, nucleus pore complex, and nanoparticle-FG protein hydrophobic affinity, we develop a coarse-grained model for the nucleus pore structure that can help us mimic and understand its process of nanoparticles' transport. We explore the roles played by nanoparticles' size, shape morphology, and surface coating in the transport process, and estimate the minimum force and energy required for a specific nanoparticle to pass through the nuclear pore complex. We believe that our findings can provide fundamental understanding in nuclear pore transport and some useful design principles for the nucleus-targeted drug delivery vectors.

14th U.S. National Congress on Computational Mechanics
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Title: Application of Atomic Force Microscopy for Investigation of Anisotropic Mechanical Properties of Living Cells

Author(s): *Chien-Kai Wang, *Tamkang University*; Ping-Liang Ko, Yi-Chung Tung, *Academia Sinica*.

The elasticity is one of the most important mechanical properties of cells because the cellular functions are highly related to their structures which can be characterized by the elasticity. Over the past decade, the atomic force microscopy (AFM) is widely applied for investigating the cellular elasticity. Through detecting the deformation causing from the applied force on cells, AFM collects the elastic modulus of cells, which are presumed to be isotropic linear elastic solids equivalently. However, it is more reasonable to consider cells to be anisotropic owing to their heterogeneous compositions. Especially, the elasticity along the substrate direction may differ a lot from the direction normal to the plasma membranes. Nevertheless, the elasticity along the substrate direction plays a particularly important role for cellular functions since cells frequently experience stretch in this direction. In implementation of bio-AFM, AFM tips are not only widely used for conventional imaging but also suitable for probing mechanical properties of living cells. The tips act as nanoindenters for the acquisition of sample elasticity through AFM measurements. At a certain spot of the cell surface, the normal force applied on a cantilever carrying the tip are consequently recorded as a function of the distance between the tip and the surface, namely, the force-displacement curve. In contact mechanics, the Hertz model considering geometrical effects and local elastic deformation properties of the indented samples has been commonly applied for interrogating the solid elasticity. In this research work, the collected force-displacement curve corresponding to each pixel of an AFM cell image is going to be processed further to yield the elastic modulus of the surface membrane along both in-plane and normal directions via optimum fit with the Hertz model of transversely isotropic solids. This study proposes a novel technique for determining the mechanical prosperities of cells along in-plane direction, helping us to understand mechanical prosperities of cells in different physiological states from a different point of view. In addition, analytical cell mechanics models are also suggested that intracellular pressure and stress distribution over cell membrane structures of various heights can be determined sequentially. Finally, we anticipate that this technique will open doors for understanding more physiological states of biological specimens under environmental loading. References: [1] Lin, C.-H., Wang, C.-K., Chen, Y.-A., Peng, C.-C., Liao, W.-H. and Tung, Y.-C. (2016). “Measurement of in-plane elasticity of live cell layers using a pressure sensor embedded microfluidic device,” Scientific Reports, 6, 36425. [2] Kuznetsova, T. G., Starodubtseva, M. N., Yegorenkov, N. I., Chizhik, S. A. and Zhdanov, R. I. (2007). “Atomic force microscopy probing of cell elasticity,” Micron, 38, 824–833. [3] Mathur, A. B., Collinsworth, A. M., Reichert, W. M., Kraus, W. E. and Truskey, G. A. (2001). “Endothelial, cardiac muscle and skeletal muscle exhibit different viscous and elastic properties as determined by atomic force microscopy,” Journal of Biomechanics, 34, 1545–1553.

14th U.S. National Congress on Computational Mechanics
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Title: Effective Properties of Cracked Multi-Domain Ferroelastic Materials under Simultaneous Straining and Thermal Cycling

Author(s): *Yun-Che Wang, Meng-Wei Shen, *National Cheng Kung University*.

Experimentally, it has been shown that the effective viscoelastic modulus and damping of ferroelastic materials, such as barium titanate, with multiple domains may be largely affected by their solid-solid phase transition, triggered by temperature variations. This observation is consistent with the theory of composite materials containing negative stiffness phases in the sense that a phase-transforming domain may be partially stabilized and interacted with the surrounding phases which have not undergone phase transition. Anomalous effective properties in metal matrix composites, containing single-domain ferroelastic particles have also been experimentally and theoretically demonstrated. However, in order not to directly use a negative modulus value in the established theories to estimate effective properties, a phase-field model is adopted in this work to directly simulate the evolution of the growth and annihilation of the ferroelastic domains that give rise to negative-stiffness effects, as stated in the Landau phenomenological theory of phase transition. The finite element method is utilized to solve the phase-field equations. Both intact and cracked ferroelastic materials are studied, and they show that the effective Young's modulus, shear modulus and bulk modulus of the multi-domain ferroelastic materials may be enhanced due to phase-transition effects. Furthermore, the overall damping of the materials, measured by the stress-strain hysteresis, may also be enhanced. Since cracks cause stress concentration near crack tips, the large stresses interact strongly with the ferroelastic phase fields, hence domains are noticeably formed around crack tips under sinusoidal straining and thermal cycling. Effects of crack tip radius on the effective properties will be discussed. In addition to modeling cracks by involving geometric empty space, such as sharp notches or penny shape cracks, we also adopt phase-field modeling techniques to simulate crack propagation in the multi-domain ferroelastic materials with the two sets of order parameters; one for the crack field and the other the ferroelastic field. The two-layer phase-field modeling enables us to study the effective properties of the ferroelastic materials during crack propagation. Moreover, contributions to the enhanced effective properties from the ferroelastic and ferroelectric phase transition will be discussed.

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Title: Efficient Uncertainty Propagation for High Fidelity Crack Growth Using Stochastic Reduced Order Models

Author(s): *James Warner, Patrick Leser, Jacob Hochhalter, *NASA Langley Research Center*.

Emerging damage prognosis approaches, such as digital twin, rely on high fidelity crack growth simulations to predict how diagnosed damage will impact a structure's future reliability. Critical to the effectiveness of such frameworks, is the quantification and propagation of inherent uncertainties resulting from measurement errors, variability in materials and loading, etc. Given the computational expense of the finite element predictions and remeshing algorithms used for crack growth modeling, using traditional Monte Carlo simulation to propagate uncertainties through these models for online damage prognosis is infeasible. To this end, this work presents a computationally efficient approach to probabilistic high fidelity crack growth using stochastic reduced order models (SROMs). Given a probabilistic description of an initial damage state and crack growth parameters, the method predicts a structure's end of life with quantified uncertainty. Numerical examples demonstrate that the SROM-based approach generates probabilistic predictions of failure in just a fraction of the time of Monte Carlo simulation while retaining a high degree of accuracy.

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Title: Finite Element Based Pelvic Injury Metric Creation and Validation in Lateral Impact for a Human Body Model

Author(s): *Caitlin Weaver, Alexander Baker, Matthew Davis, Joel Stitzel, *Wake Forest School of Medicine*; Anna Miller, *Washington Univ, Dept. of Orthopaedic Surgery*.

Pelvic fracture is a very serious injury resulting in a high risk of mortality and resulting morbidity. This injury can be caused by low energy trauma or high energy trauma. Mortality and morbidity risk from pelvic fracture vary depending on the type of pelvic fracture. The purpose of this study is to develop injury risk prediction curves for specific regions of the pelvis by comparing the presence of fracture in these regions in experimental testing to the cross-sectional force response in these regions in a total human body FE model. The total human body FE model used for this study was Global Human Body Models Consortium (GHBMC) 50th percentile detailed male FE model (v4.3). Lateral impact FE simulations were performed using input data from lateral impact tests performed by Bouquet et al. on post mortem human subjects (PMHS). The simulations were scaled using five normalization techniques. These techniques were validated using log rank testing, Wilcoxon rank sum testing, and correlation and analysis (CORA). Survival analyses were performed on the experimental test data and the simulation test data (scaled and unscaled) to generate injury risk prediction curves for total pelvic injury. This method was used to generate injury risk prediction curves for regional pelvic injury. Pelvic injury risk prediction curves were developed for total pelvic injury risk using applied force and regional pelvic injury risk using cross-sectional force. The results show good correlation for total pelvic injury risk prediction between the experimental and simulation data with most normalization techniques. Based on results from the log rank, Wilcoxon, and CORA analyses, the equal stress equal velocity (ESEV) scaling method was determined to be the best normalizing technique for this study. The injury risk prediction curve generated from the scaled simulation data shows slight under prediction of injury in comparison to the experimental data curve, however, this difference was determined to not be statistically significant. Injury risk curves were developed for the inferior pubic rami, superior pubic rami, and the sacroiliac region using cross-sectional forces from the simulation results and the occurrence of injury documented in the experimental autopsies. The work performed in the paper provides a robust tool for determining risk of pelvis fracture in the FE environment. The injury risk prediction methods developed in this study analyze injury metrics on a local level based on fracture location as well as on a component level (i.e. axial vs. shear vs. resultant).

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Title: An Image Based Finite Element Model for Ni-Based Superalloys Using a Two Scale Constitutive Model Accounting for Morphological Distributions of Gamma' Precipitates

Author(s): *George Weber, Maxwell Pinz, Akbar Bagri, Somnath Ghosh, *Johns Hopkins University*.

A polycrystalline crystal plasticity finite element model is developed for γ-γ' nickel-based superalloys with constitutive behavior established over two length scales. A dislocation density-based crystal plasticity model, at the scale of subgrain microstructures containing γ' precipitates in a γ-matrix within a single crystal, is implemented to include the effects of dominant thermo-mechanical micromechanisms. However, due to the large number of γ' precipitates per grain, it is computationally expensive to incorporate explicit γ-γ' microstructures for polycrystalline crystal plasticity simulations of these alloys. Thus, a parametric homogenization scheme is pursued to develop a single crystal homogenized constitutive law accounting for the morphology of the precipitate-matrix substructure without explicitly representing the two phase geometry. To this goal, a series of γ-γ' statistically equivalent representative volume elements (SERVEs) are generated to understand the sensitivity of the micromechanical response to various distributions of local geometric features of the precipitates such as local volume fraction, two-point correlation function, precipitate shape parameterization, and local descriptions of channel width. Tools in global sensitivity analysis and uncertainty quantification are utilized to determine the most important of these microstructural features that must be translated to the next scale. The homogenization of the subgrain SERVEs yields a single crystal constitutive law with a functional dependence on these inherent microstructural distributions. Each of the statistical representations of the morphological quantities is derived from and compared to experimentally gathered distributions resulting from image analysis of serial sectioned SEM data. This multi-scale image-based framework is implemented to study the performance of polycrystalline microstructures under constant strain rate loading, creep, and fatigue. Through variation of homogenized distribution parameters, the effect of subgrain morphological statistics can be connected to microstructural design at the polycrystalline length scale.

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Title: Multi-Objective Optimization of Multi-Scale Finite-Element Analysis for Wear Resistant Steel

Author(s): *Peerapon Wechsuwanmanee, Junhe Lian, Sebastian Münstermann, *RWTH Aachen University*.

In wear resistant steel production, hardness is one of the most crucial property to be considered. Nevertheless, toughness is always its trade-off. Due to the fact that microstructure features, e.g. grain size, influence these mechanical properties, this work proposes a multi-objective optimization scheme to achieve optimal artificial microstructure which delivers high hardness while maintaining toughness. Firstly, the existing material is characterized. Finite-Element (FE) models in macroscopic level are then constructed and validated by charpy test and Vicker hardness test. A homogenization method is applied to bridge the macroscopic level into the microscopic level. A representative volume element (RVE) model with the existing material's microstructure is obtained and implemented on the virtual experiment scheme. Once the multi-scale model from existing material is achieved, a well-known multi-objective optimization approach namely particle swarm optimization (PSO) is employed in order to acquire the optimal artificial microstructure.

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Title: Efficient High Fidelity Nonlinear Dynamic Analysis of Light Gauge Steel Walls Subjected to Blast Loading

Author(s): Ahmed Khalil, *Applied Science International* ; Nabil Rahman, *The Steel Network Inc.*; Matt Whelan, *David Weggel, *University of North Carolina, Charlotte*.

This paper presents modeling results for a series of full-scale open arena blast tests of curtain wall light gauge steel panel systems developed by The Steel Network, and tested by the University of North Carolina, Charlotte to validate the blast resistance capabilities of the system especially the head-of-wall and bridging connections. The wall tests were modeled using two high fidelity nonlinear dynamic techniques: the finite element method and the applied element method. The tests subjected the test walls to blast impulse values that are higher than the minimum Unified Facility Criteria values as specified in UFC 3-340-022, “Structures to Resist the Effects of Accidental Explosions” and UFC 4-010-023, “DoD Minimum Antiterrorism Standoff Distances for Buildings”. The ductility values for the test walls were calculated from the tests as the ratio of maximum displacement to yield displacement. The wall tests were modeled using the Applied Element method and the Finite Element method. The materials models used to model the walls were nonlinear steel model for the steel studs as well as a bilinear material model for plywood sheathing. The results of the nonlinear dynamic time history analysis of the walls are summarized and compared. Additionally, recommendations are presented on optimizing the computational requirements while still maintaining acceptable agreement with the experimental results. The ductility values observed in the tests and the analytical models were more than four times the requirements by U.S. Army Corps of Engineers Protective Design Center (PDC) for the design of top slip track studs walls and twice that the requirements for studs connected top & bottom. The tests and the high fidelity numerical models showed that the head-of-wall TSN VertiClip® connection and the TSN BuckleBridge® bridging system kept the wall intact and allowed the studs to develop the required ductility under the effect of the blast loading.

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Title: Multidisciplinary Topology Optimization Using Hierarchical Distributed Computing

Author(s): *David Weinberg, *Autodesk, Inc.*; Nam-ho Kim, *University of Florida*.

For last thirty years, topology optimization has significantly been developed in engineering design. Different from conventional parameter or shape design, topology optimization can provide important insights on design. Starting from a maximizing stiffness (minimizing compliance) design, now topology optimization can be applied to various other disciplines. Due to complexity in engineering design, most industrial design problems are multidisciplinary in nature, where different physical phenomena are involved in a single design formulation. For example, in aerospace applications, the stiffness, buckling and heat transfer performances need to be considered simultaneously. Therefore, it is important that topology optimization can handle multidisciplinary optimization. In this presentation, the concept of distributed computing is utilized to solve multidisciplinary topology optimization problems using Autodesk Nastran. The idea is to distribute simulations in different disciplines to different processors, which is the first level of distributed computing. Next, the individual discipline simulation can also be distributed to multiple processors in the conventional notion of distributed computing. Therefore, the framework is a hierarchical distributed computing. When the optimization engine is a main program, and it calls different finite element simulations based on disciplines, the distributed computing can be straightforward. However, in the current software architecture [1], finite element simulation is a main program and optimization is a subroutine to update design variables at each iteration. In such a case, the distributed computing for optimization is not straightforward. The current architecture assumes that the design problem has a single objective function with multiple constraints using different disciplines. The main topology optimization engine is controlled by the independent processor, while constraints in different disciplines are controlled by dependent processors. All different disciplines need individual model input files, but all models need to have the same mesh and number of elements in the topology optimization design space. All input files are launched individually in different command lines. Once all dependent processes finish simulation and calculate adjoint sensitivity, the independent process continues to running the main topology optimization engine. This process is repeated until the main topology optimization engine converges. The presentation will show how multidisciplinary constraints can affect the optimum design. The presentation also shows the current progress on automatically converting topology optimization results to the smooth boundary and to the CAD model. [1] D. Weinberg and N. H. Kim, Experiences of software development for topology optimization, The 12th World Congress on Computational Mechanics, 24-29 July 2016, Seoul, Korea

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Title: Coupling Fracture Propagation and Reservoir Simulator

Author(s): *Mary Wheeler, Benjamin Ganis, Mohamad Jammoul, Sanghyun Lee, *University of Texas at Austin*.

Natural and hydraulic fractures act as major heterogeneity in the subsurface that control flow and transport of subsurface fluids and chemical species. Both flow in fractures and fracture propagation can have important effects on transmissivity, and can impact migration during applications such as geologic sequestration of CO2 and oil and gas production. Advanced computational methods are critical to design subsurface processes in fractured media for successful environmental and energy applications. This talk will present one such advanced computational method for coupling hydraulic fracturing with reservoir simulator to perform efficient multi-scale and multi-physics simulation of flow, geomechanics, and fracture propagation. The fractures are represented by a diffuse phase-field variable, whose growth is determined by the solution of partial differential equations arising from an energy minimization functional. The fluid flow is modeled using a multiphase multicomponent equation of state compositional model by our in-house reservoir simulator IPARS (Integrated Parallel Accurate Reservoir Simulator). We emphasize the computational technique to integrate small scaled hydraulic fractures to a large scale reservoir domain. Computational algorithms including data management, mesh refinement, and parallelization for high performance computing will be discussed.

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Title: A Spatial Clustering Algorithm for Constructing Local Reduced-Order Bases for Nonlinear Model Reduction

Author(s): *Tina White, Phil Avery, Charbel Farhat, *Stanford University*.

Projection-based Model Order Reduction (PMOR) techniques rely on the precomputation of an approximation subspace that, despite having a dimension much smaller than that of its underlying high-dimensional model, exhibits the ability to capture its dominant features. Compressing a matrix of solution snapshots using SVD is a widely used method for constructing such a subspace. However, for highly nonlinear problems characterized by distinct physical features and/or scales, a global application of this method cannot be expected to produce a Reduced-Order Basis (ROB) with the smallest possible dimension. A new approach for adressing this issue is the method of local ROBs introduced in [1]. There, the solution space is first partitioned into subregions using a clustering algorithm applied to the columns of the snapshot matrix. Local ROBs are then constructed and assigned to the various subregions. Although this approach has demonstrated a significant potential for achieving large speedups while maintaining good accuracy, it has room for improvement, particularly for problems characterized by spatially varying features and/or scales. To this end, a complementary method for constructing local ROBs is presented here. The solution space is first partitioned into subregions by clustering not only the columns of the snapshot matrix, but also the rows of each column-wise snapshot cluster. Local ROBs are then constructed and assigned to the various subregions. Row-wise clustering allows PMOR to leverage information regarding spatial structures that may be encoded in the snapshot matrix. It also furnishes a natural mechanism for capturing multiscale phenomena. The proposed method is amenable to existing hyper reduction techniques such as GNAT [2] and ECSW [3]. Hence, it admits a computationally efficient implementation that is demonstrated here.

14th U.S. National Congress on Computational Mechanics
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Title: Multilevel Decomposition and Compression on Unstructured Grids

Author(s): Mark Ainsworth, *Ben Whitney, *Brown University*.

Large scale simulations regularly produce terabytes or even petabytes of data. The scale of these datasets complicates post hoc analysis and can render the sharing of data between different research centers prohibitively expensive. Hierarchical decomposition schemes promise a partial solution to these problems. In such schemes, the data to be analyzed is split into a number of components, which may be distributed across heterogeneous storage media and can be selectively recombined to produce approximations to the original data of varying levels of accuracy. Hierarchical methods in use today include ad hoc methods such as decimation (analyzed in [Ainsworth et al. 2017]) and wavelet methods for structured grids. In this talk, we introduce and analyze a simple decomposition scheme based on $L^2(\Omega)$ projections that is suitable for unstructured grids. We show that the scheme is quasioptimal in its use of storage and discuss its efficient implementation, including integration with the IO system ADIOS. We conclude with representative numerical examples and a discussion of further extensions.

14th U.S. National Congress on Computational Mechanics
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Title: Adaptive Multiscale Modeling Using Generalized Mortar Methods

Author(s): *Tim Wildey, Bart Van bloemen waanders, Tom Seidl, *Sandia National Labs*.

Multiphysics systems are typically strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a large range of length- and time-scales. Performing direct numerical simulation of such systems that resolves all of the relevant length- and time-scales is often prohibitive, even on the modern leadership-class computing platforms. Consequently, we are interested in developing multiscale methods to allow the incorporation of fine scale information into a coarse scale approximation. The process of injecting information from unresolved, or subgrid, scales into a coarse scale discretization has been pursued in several different ways by different communities. Many of the existing approaches are based on computational homogenization where the objective is to define model parameters on the coarse grid in a consistent manner so that the coarse scale solution is a reasonably accurate numerical approximation of the fine scale solution. While tremendous progress has been made both theoretically and computationally, the process usually requires rather strict assumptions, such as periodicity of the media, and is difficult to generalize to multiphysics applications. In this presentation, we describe our recent efforts to generalize the multiscale mortar method to provide a concurrent multiscale approach for multiphysics systems that does not rely on homogenization. We describe some of the similarities between our mortar-based approach and existing methods, e.g., the variational multiscale method, the hybridizable discontinuous Galerkin method, and the multiscale discontinuous Galerkin method. We also describe the dynamic adaptive multiscale capability that we recently developed using Trilinos. Numerical examples will be presented to illustrate the benefits in using the generalized multiscale mortar approach for a variety of applications.

14th U.S. National Congress on Computational Mechanics
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Title: A Class of Mixed Finite Element Methods for the Compressible Navier-Stokes Equations

Author(s): *David Williams, *Pennsylvania State University*.

How can we continue to create more accurate and robust methods for solving the compressible Navier-Stokes (NS) equations? This is a fundamental challenge facing numerical analysts, as in many instances, accuracy and robustness are in opposition to one another. In this talk, we propose a class of methods that have the potential to avoid the standard tradeoffs between accuracy and robustness. The proposed class of mixed finite element methods employs high-order polynomial basis functions to facilitate accuracy, and residual-based stabilization techniques to facilitate robustness. It is anticipated that the resulting methods will be well-suited for producing high fidelity solutions to the compressible NS equations under difficult circumstances, and in particular, on highly distorted, solution-adapted meshes. This is of paramount importance, as the practical geometries of interest continue to become more complicated. As the trend continues, engineers can no longer reliably generate quality meshes based on physical insight, and mesh adaptivity becomes a necessity, in conjunction with numerical methods that perform robustly on adapted meshes.

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Title: Exact Transfer- and Stiffness Matrix for the Composite Beam-Column with Refined Zigzag Kinematics

Author(s): *Heinz Wimmer, *HTL-1 Linz*; Karin Nachbagauer , *U. Appl. Sci. of Upper Austria*.

The Refined Zigzag Theory (RZT), developed by Tessler/Di Sciuva/Gherlone is among the most promising approaches for analyzing composites structures today. Since its appearance many contributions have been published dealing with finite elements for laminated structures based on the efficient kinematic of RZT. For composite beam-columns C0-elements of different orders [1] as well as p-type approximations [2] are formulated and assessed. In this work a different approach is given. After establishing the governing equations in a first order differential equation system the transfer matrix is obtained by a matrix series solution. The transfer matrix approach, in principle suited for 1D-structural elements such as beams, disks, circular plates and rotational shells, has successfully applied in the past [3]. Sometimes this approach exhibits numerical instabilities. The well-known relations between the transfer- and stiffness matrix are invoked to circumvent this drawback. The dynamic stiffness matrix and the load vector are obtained by reordering and partially inverting the sub matrices of the transfer matrix. The results, which are obtained by one finite element only, are in agreement with available analytical und numerical solutions. For practical applications a combined usage of both types of matrices makes sense. [1] Di Sciuva M. et al.: A class of higher-order C0 composite and sandwich beam elements based on the Refined Zigzag Theory. Composite Structures 132 (2015), 784-803. [2] Nallim L.G. et al.: A hierarchical finite element for composite laminated beams using a refined zigzag theory. Composite Structures 163 (2017), 168-184. [3] Wunderlich W., Pilkey W.D.: Mechanics Structures. Variational and Computational Methods. CRC Press 2003.

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Title: Using a Sponge Layer as a Boundary Treatment for Open-Ocean Boundaries in a Finite-Element-Based Coastal Ocean Model

Author(s): *Damrongsak Wirasaet, William J. Pringle, Andika Suhardjo, Joannes J. Westerink, *University of Notre Dame*; Juan Gonzalez, *Caribbean Coastal Ocean Observing System*.

Open-ocean boundary conditions, which are required to complete the model description on the ocean side, have large effects on the solution of numerical coastal flow modeling. It is important that the open-ocean boundary conditions introduce only desired information into the domain and minimize reflection of outgoing waves. One of the most widely used conditions simply imposes a surface water level. Although sufficient to some degree for the former purpose, this condition generally reflects a component of outgoing waves and may introduce unwanted numerical artifacts. In this study, we investigate the use of a sponge layer as an alternative treatment for open-ocean boundary conditions in the context of a massively-parallel continuous finite-element-based shallow water flow model. Numerical experiments using a set of numerical tests, ranging from an idealized model problem to a realistic tidal flow, show that the sponge layer treatment provides satisfactory results and improves the robustness of the numerical model significantly.

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Title: On the Impact of Number Representation for High-Order Implicit Large Eddy Simulations

Author(s): *Freddie Witherden, Antony Jameson, *Stanford University*.

High-order numerical methods for unstructured grids combine the superior accuracy of high-order spectral or finite difference methods with the geometric flexibility of low-order finite volume or finite element schemes. Over the past few years they have shown promise in enabling implicit large eddy simulations within the vicinity of complex geometrical configurations. However, the cost of such simulations remains prohibitive. At the same time there has been a steady increase in the ratio of single to double precision performance in contemporary hardware platforms; which can be as high as 32:1. This suggests that one means of reducing the cost of such simulations and/or improving the time to solution is to migrate to single precision. In this presentation we consider the impact of number representation on the efficiency and efficacy of these methods. Implementation issues will be discussed. Theoretical performance models will also be derived and assessed using four standard test cases i) an isentropic Euler vortex, ii) the viscous Taylor–Green vortex, iii) flow over a circular cylinder, and iv) flow through a T106c low pressure turbine cascade. We shall detail findings which indicate that, with the exception of the isentropic Euler vortex test case, the exclusive use of single precision arithmetic has no meaningful impact on accuracy.

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Title: Designing Morphology Evolution Pathways in Organic Thin Films

Author(s): Prosenjit Bhattacharya, *Olga Wodo, *University at Buffalo*.

Organic thin films have the potential to revolutionize next generation of organic electronic (OE) devices as it exhibits flexibility, stretchability, softness and compatibility with biological systems – features traditionally missing in silicon-based solutions. Almost from its inception, OE has ignited the imagination to build devices covering a whole spectrum of technologies ranging from transistors, solar cells, diode lighting and flexible displays to integrated smart systems such as RFIDs, smart textiles, artificial skin, and implantable medical devices and sensors. Its promise is fueled by an ability for cheap and rapid roll-to-roll fabrication, compatibility with flexible substrates, high optical absorption coefficients, low-temperature processing, and easy tunability by chemical doping. However, many promising OE technologies are still bottlenecked at the process optimization stage – more specifically, at designing processing pathways that result in tailored morphology. Current state-of-art approaches are primarily Edisonian – trial-and-error experimental approaches – that only explore a very narrow slice of the processing space due to resource and time constraints. This is further exacerbated by a glaring lack of comprehensive knowledge about the influence of processing pathways on morphology evolution as well as the link between processing pathways and device characteristics. In this work, we focus om solvent-based fabrication of organic thin films. Solvent-based thin-film deposition technologies (e.g. spin coating, drop casting, doctor blading, roll-to-roll manufacturing) are the most common OE manufacturing techniques. All solution-processing techniques usually involve preparing dilute solutions of polymers in a volatile solvent. After some form of coating onto a substrate, the solvent evaporates. An initially homogeneous mixture separates into polymer-rich regions as the solvent evaporates. Depending on the specifics of the polymer blend and processing conditions (e.g. evaporation rate, solvent type, nature of substrates), different morphologies are typically formed. Multitude of process and system variables makes exploration of the corresponding parameter space impractical. To rank order manufacturing variables, we perform the sensitivity analysis of the main governing equations. For each process and system variables, we will execute our computational model to track morphology evolution under given input parameters, and record the morphology evolution path. This work has important implications to navigate smart exploration of processing space and ultimately to facilitate design of manufacturing of organic electronics devices with improved properties.

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Title: A Linear Sampling Method for Through-the-Wall Radar Detection

Author(s): Matthew Charnley, *Rutgers University*; *Aihua Wood, *Air Force Institute of Technology*.

The through-the-wall inverse scattering problem is analyzed via the linear sampling method. The reciprocity gap formulation of the linear sampling method is used to reconstruct an object within a closed-off room. In order to apply this method, a numerical method to model a point source is needed, along with knowledge of how the numerical fundamental solution differs from the analytic one. Application of the linear sampling method to the Finite Difference Time Domain solution is described and illustrated, and results to reconstruct objects in the through-the-wall setting are shown.

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Title: Interfacing Geotechnical and Hydrodynamic Models to Resolve Failure Mechanisms of Flood Control Systems under Storm Surge

Author(s): *Dylan Wood, Ethan Kubatko, Abdollah Shafieezadeh, Mehrzad Rahimi, *The Ohio State University*.

Modeling of storm surge or similarly extreme flow events provides valuable information to decision makers so that they may act to mitigate risk. Of considerable concern to decision makers is the ability of flood defense systems to withstand these extreme flow conditions. Current hydrodynamic models, such as ADCIRC and DG-SWEM, are limited in the scope of data they provide on flow-structure interaction, wherein only one failure mechanism may be resolved for flood systems (overtopping), though in reality various geotechnical failure mechanisms are possible. We present efforts towards interfacing current shallow-water based hydrodynamics models with geotechnical results from a three dimensional fully coupled fluid-particle model to simulate flood-induced seepage, and to study our ability to resolve this mechanism's contribution to flood control failure during large scale flood events. We verify our results for several test cases and compare them to those obtained with previous hydrodynamic models.

14th U.S. National Congress on Computational Mechanics
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Title: A Novel Constraint Enforcement Method for Implicit Contact Mechanics

Author(s): *Steven Wopschall, Mark Rashid, *UC Davis*.

The implicit solution to quasi-static contact problems in nonlinear solid mechanics poses many challenges. A primary difficulty is the enforcement of the contact inequality constraints. Using a new contact formulation based on a median-plane methodology with integral-form gap constraints, a novel contact enforcement procedure is introduced. This procedure uses a subcycling method that simultaneously handles active and inactive constraints, thus circumventing limitations associated with active set strategies, and difficulties posed by methods relying on heuristics or user action. Handling complex contact interfaces in the presence of geometric and material nonlinearity, this method results in kinematically admissible, and physical, contact solutions for difficult implicit quasi-static contact problems.

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Title: Parallelization of Numerical Integration Algorithm for rIGA Using a Fast Quadratures

Author(s): *Maciej Wozniak, Maciej Paszynski, *AGH UST*.

The three-dimensional isogeometric analysis (IGA-FEM) computations over a patch of elements involve the generation of the system of linear equations followed by the solution performed by either iterative or direct solver. In this talk, we focus on speeding up the integration phase, and we compare its costs to the cost of the solution of the resulting system of linear equations by using multi-frontal direct solver algorithm. We utilized the refined isogeometric analysis (rIGA) [1] which introduces C0 separators between patches of higher continuity elements in order to reduce the computational cost of the multi-frontal direct solver. It results in optimal sparsity pattern of the matrix structure which in turn speeds up direct solvers. Both standard IGA and rIGA methods come with challenging sparse matrix structures, that is expensive to generate. Sequential integration for rIGA FEM method takes the substantial part of the total computational cost. New quadratures dedicated for IGA FEM have been developed [2]. They allow reduction of quadrature points by one magnitude compared to traditional Gaussian quadratures. In this paper, we utilize the new quadratures to speed up the rIGA computations. We also propose a hybrid parallelization method to reduce the computational cost of the integration phase using hybrid-memory parallel machines and new quadratures. The two-level hybrid parallelization includes the domain decomposition on the first level and loop parallelization on the second level. We employ hybrid MPI plus OpenMP implementations. We show that our hybrid parallelization of the integration reduces the contribution of this phase below one percent of the total execution time when dealing with parallel direct solvers with rIGA. Thus, the integration phase is no longer an issue when dealing with multi-frontal direct solvers. The proposed hybrid parallelization can be applied for both IGA and rIGA codes. Acknowledgment, The work of Maciej Wozniak, has been supported by Dean's grant from Faculty of Computer Science, Electronics, and Telecommunication, AGH University, Krakow, Poland. The work of Maciej Paszynski has been supported by National Science Centre, Poland grant no. 2016/21/B/ST6/01539. [1] Daniel Garcia, David Pardo, Lisandro Dalcin, Maciej Paszy■ski, Nathan Collier, Victor M. Calo, The Value of Continuity: Refined Isogeometric Analysis and Fast Direct Solvers, Computer Methods in Applied Mechanics and Engineering, 316 (2017) 586-605 [2] Michael Barton, Victor Calo, Optimal quadrature rules for odd-degree spline spaces and their application to tensor-product-based isogeometric analysis, Computer Methods in Applied Mechanics and Engineering, 305 (2016) 217-240

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Title: Static and Dynamic Applications of Atomistic-Based Boundary Element Method

Author(s): *Xiaojie Wu, Xiantao Li, *Penn State University*.

Atomistic-based Boundary Element Method (ABEM) is a novel technique to seek the exact solution for harmonic solids. Due to the lattice Green's function, all the atoms inside the domain are eliminated. And the number of DOFs is significantly reduced. Also, ABEM in Laplace domain turns out to be suitable to simulate time-dependent problems. Because of the harmonic assumption, ABEM itself is not able to simulate the solid system with defects. But ABEM can be naturally coupled with the standard atomistic simulation. The coupling approach can be applied to many problems from material science. Numerically, the number of DOFs can be further reduced by introducing boundary elements where the displacement field is smooth. The linear system is built by a fast summation technique. Both static coupling and dynamic coupling are verified by comparing the results with full molecular simulations. Further numerical experiments are performed to show the capability of the approach.

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Title: A Robust Particle Gakerkin Method for High-Speed Metal Grinding Simulation

Author(s): *C.T. Wu, *LSTC*.

In this study, we present a particle Galerkin method for the simulation of high-speed metal grinding process. The present numerical method begins with an establishment of a stabilized and regularized particle Galerkin approximation. A non-residual penalty term from strain smoothing is introduced as a means of stabilizing the particle Galerkin method. Additionally, the second-order strain gradients are introduced to the penalized functional for the regularization of damage-induced strain localization problem. To handle the severe deformation in metal grinding simulation, an adaptive anisotropic Lagrangian kernel is employed. Finally, the formulation incorporates a bond-based failure criterion to bypass the prospective spurious damage growth and material self-healing issues in material failure simulation. A three-dimensional metal grinding problem is analyzed and compared with the experimental result to demonstrate the effectiveness of the proposed numerical procedure.

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Title: Open Source, Tightly Coupled, Partitioned Fluid-Structure Interaction Simulation Capability for High Spatiotemporal Resolution During Study of Wave Impact Loads in High Speed Watercraft

Author(s): *Wensi Wu, Justyna Kosianka, Christopher Earls, *Cornell University*.

The present work is aimed at using computational tools to study the very challenging Fluid-Structure Interaction (FSI) problem known as “slamming.” Slamming occurs when shell surfaces, comprising the outer skin on the hull of high speed watercraft, impact the water in a way that has the shell normal nearly orthogonal to the water free surface. Such loading results in water jets, spray sheets, multi-phase and breaking flows on the fluid side along with very high strain rates and very nonlinear responses on the structures side. Additionally, the density of the fluid is on the same order as the density of the structure, and so the resulting FSI is very tightly interacting, and any simulation of such an FSI context must respect this situation; thus requiring implicit coupling schemes. The current presentation describes a modeling framework that effects an implicit, partitioned coupling of an open source computational fluid dynamics (CFD) tool (OpenFOAM) to an open source computational structural dynamics (CSD) tool (CU-BEN) in order to effectively treat the anticipated physics at play within the problem of slamming. The resulting forward modeling tool will be validated using a series of very carefully conducted experimental tests by our collaborators, and the validated models will then be applied to developing better instrumentation for additional, subsequent experimental work. In this way, we will study the slamming problem as an exercise in computational science and engineering (CSE), where the computational tool is vital to simulate physical system with fidelity that has been hitherto unrealizable within the laboratory setting, so that more sophisticated experimental methods can be developed, and the physical phenomenon better understood.

14th U.S. National Congress on Computational Mechanics
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Title: Node Creation for Isotropic Refinement of Tetrahedral Meshes

Author(s): *Nick Wyman, Steve Karman, *Pointwise, Inc.*.

Refinement of tetrahedral meshes to support user-prescribed or simulation-driven distribution of element sizing requires the creation of interior nodes for insertion into the mesh. Interior node count and location is a balance of mesh efficiency and quality as well as solution robustness, efficiency, and accuracy. While mesh efficiency and refinement termination guarantees are possible in 2D, the authors are unaware of any such guarantee in 3D. Additionally, mesh efficiency is seldom the most important feature of a production oriented meshing algorithm. The authors present two methods for determination of candidate interior points for mesh refinement and contrast their computational performance during mesh generation and CFD simulation. The first method is an ad hoc edge subdivision scheme (locally 1D) while the second is a novel physics-based simulation in 3D. The edge subdivision scheme generates a set of candidate nodes for a given edge within the mesh. Within the 1D framework of the edge, the candidate node count and distribution is optimized to satisfy prescribed edge length and edge length gradation goals. Edges are processed in a priority queue resulting in a queue of candidate nodes to be added to the mesh, some of which may be equivalent w.r.t. local element size. In our approach the candidate node queue is efficiently pruned of equivalent nodes via tree data structures and by minimizing queue size. Candidate nodes are inserted into the mesh and edge subdivision repeated until all edges are within tolerance of the prescribed local element size. A second method of interior node creation is based on inter-particle (inter-node) force interactions that distribute the nodes smoothly across the interior. The force model includes an attractive force when nodes are farther apart than the prescribed element size and a repulsive force when nodes are too close together. All nodes can influence all other nodes, but they generally only influence nodes within a specific radius of the central node. Periodically the set of nodes is evaluated, based on overlap ratio, to determine if node insertion and deletion is necessary. The converged interior node system is then inserted into mesh. Example 3D cases, both simple and complex, will be shown which demonstrate the mesh smoothness that results from the physics-based approach compared to the edge subdivision approach. Results of CFD solutions utilizing meshes created with the two refinement schemes will be compared.

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Title: Towards a Meshfree Finite Difference Model for Reactive Mixing Problems

Author(s): *Timo Wächtler, Jörg Kuhnert, *Fraunhofer ITWM*.

The Finite Pointset Method (FPM) [1] -developed and implemented at Fraunhofer ITWM- is a meshfree finite difference method for the numerical solution to problems in continuum mechanics such as fluid flows. In FPM, the finite set of computation nodes (point cloud) moves along the trajectory of the fluid flow (lagrange coordinates) and the meshfree character of the method allows to easily adapt the point cloud to changes in the domain of computation such as the movement of free surfaces or rapid geometry movement, e.g. a rotating stirrer. Over the last decade, the software package has been applied successfully to several problems in industry such as processes of water crossing, sloshing and filling. The software package and the method are under continuous development and in pursuit of new types of application for FPM, this contribution will present fundamentals of the method and the current state of an FPM model for simulating processes of reactive mixing. Such processes are fundamental operations in chemical engineering and simulations are required in that context to design the mixing devices, in particular to improve the process of the scale-up from laboratory scale to industrial scale. [1] J. Kuhnert, Meshfree Numerical Scheme For Time Dependent Problems in Fluid and Continuum Dynamics, S. Sundar (Ed), ADVANCES IN PDE MODELING AND COMPUTATION, Ane Books Pvt. Ltd, p. 119-136, 2014 . [2] Tiwari S., Kuhnert J., Finite pointset method based on the projection method for simulations of the incompressible Navier-Stokes equations, M. Griebel, M. A. Schweitzer (Eds.), Springer LNCSE: Meshfree Methods for Partial Differential Equations, Springer-Verlag, Berlin, 26, p. 373-387, 2003

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Title: Fully Resolved Numerical Simulations of Fused Deposition Modeling

Author(s): *Huanxiong Xia, Jiacai Lu, Gretar Tryggvason, *University of Notre Dame*; Sadegh Dabiri, *Purdue University*.

Fused Deposition Modeling (FDM) is one of the most common additive manufacturing processes. In FDM, complex three-dimensional objects are built by depositing filaments of hot polymers that fuse together when they solidify. Free extrusion, a moving interface and solidification are the distinctive features of the FDM process, leading to numerous challenges for understanding the physical behaviors and parametric effects in the numerical simulations. Here we describe preliminary development of a fully resolved model and examination of the various features of the FDM process. In our model, the process is embedded in a hexahedral computational domain and the system is treated as two-phase immiscible fluid flow, where the main body and the moving interface are discretized using structured and unstructured grids, respectively, using a finite volume/front tracking method. The extrusion of the polymer is modelled as a moving volume source that follows a prescribed trajectory. The viscosity depends on the temperature and the shear rate of the polymer, and solidification is captured by the rapid increase of the viscosity of the polymer. For materials used in the FDM process the high ratios of the values of the material properties between the air and the melt pose numerical challenges. Here we have implemented an implicit scheme for the viscous terms in the momentum equation and the thermal diffusive term in the energy equation to meet these challenges. A convergence study, including four different levels of grid resolutions, was carried out to test the accuracy of the model. The contact area between the two neighboring filaments and the volumetric average temperature indicated that the results had converged for the benchmark resolution. We also show a simulation of a representative object, where the top filaments were laid down either parallel or perpendicular as the one in the adjacent layer, to demonstrate the capabilities of the method. The effects of the nozzle velocity on the shape of the filament and the injection temperature on the reheated depth were examined, and those, along with other aspects of the process will be discussed.

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Title: Experimental Measurement of Contact-Line Mobility Using Drop Resonance

Author(s): *Yi Xia, Paul Steen, *Cornell University*.

Contact-line mobility characterizes how fast a liquid can coat a solid support. During rapid movement of liquid across a solid, the dynamical contact angle changes in response to changes in contact line speed. Mobility captures this far-from-equilibrium behavior. For sufficiently rapid movement, the flow is largely inviscid and surface tension and liquid inertia compete to influence the interface shape near the support. We use a mechanical oscillator to induce resonance in a supported liquid drop and generate resolvable contact line motions. The mobility parameter is then extracted from measurements of contact line displacement, contact line speed and contact angle.

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Title: Solving Large-Scale Nonlinear Eigenvalue Problems in Boundary Element Method by Resolvent Sampling Based Rayleigh-Ritz Method

Author(s): *Jinyou Xiao, *Northwestern Polytechnical Uni*; Junpeng Wang, Tao Wang, Lihua Wen, *Northwestern Polytechnical University*.

Numerical solution of large-scale nonlinear eigenvalue problems (NEPs) in the boundary element method (BEM) is an important task in many branches of the BEM-based engineering simulation and design. However, it remains a challenging task to date due to the lack of reliable and effective numerical methods. In this talk, the recently developed resolvent sampling based Rayleigh-Ritz projection method (RSRR) [1,2] is adoped to solve large-scale NEPs in the BEM. It consists of two steps: first, constructing an eigenspace by solving frequency-domain BEM systems at a series of sampling frequencies with given right-hand-side vectors, and then, projecting the original NEP onto the eigenspace and solving the reduced small-scale NEP by existing methods. There are two crucial issues that can significantly affect the computational efficiency of the RSRR. In the first step, when the sampling frequencies approach some of the unknown eigenvalues, the BEM matrices become nearly singular and iterative linear system solvers will be difficult or fail to converge. In the second step, the solution of the reduced NEPs usually requires to compute the original BEM matrices hundreds or thousands of times, which is computationally prohibitive in large-scale simulations. To settle the former issue, an additive preconditioning technique leading to well-conditioned system matrices is proposed, and a combined preconditioner is proposed as well to further accelerate the convergence rate of the resultant linear systems. For the latter issue, the original BEM matrix is interpolated using the discretized Cauchy integral formula, which leads to an explicit expression of the reduced system matrix, so that the computation of the original BEM matrices is completely avoided in solving the reduced NEPs. The method is used to solve practical acoustic modal analysis problems. Complicated sound absorbing boundary conditions and large-scale examples with more than 0.4 million degrees of freedom are considered. Numerical results show that the RSRR method can robustly dig out all the interested eigenpairs with good accuracy and high computational efficiency. References: [1] Xiao J, Meng S, Zhang C, et al. Resolvent sampling based Rayleigh–Ritz method for large-scale nonlinear eigenvalue problems. Computer Methods in Applied Mechanics and Engineering, 2016, 310: 33-57. [2] Xiao J, Zhang C, Huang T M, et al. Solving large■scale nonlinear eigenvalue problems by rational interpolation and resolvent sampling based Rayleigh–Ritz method. International Journal for Numerical Methods in Engineering, 2016.

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Title: A Local Discontinuous Galerkin Finite-Element Method for the Richard's Equation

Author(s): *Yilong Xiao, Ethan Kubatko, *The Ohio State University*.

Unsaturated flows in porous media arising from hydraulic conductivity, capillary pressure and gravity are governed by the Richards' equation. Most past numerical Richards' equation solvers were based on finite difference or continuous Galerkin finite element methods (CG-FEM). In the context of the latter, the requirement on solution continuity can lead to numerical difficulties when abrupt change occurs in boundary conditions or in hydraulic properties of the porous media. In light of these challenges, a one-dimensional numerical Richards' equation solver is formulated based on the local discontinuous Galerkin finite element method (DG-FEM) – a class of finite element methods that employs piecewise continuous trial spaces and allows discontinuity in solutions, which can better accommodate high-intensity moisture inputs and natural heterogeneities. Soil moisture readings we obtained under controlled laboratory settings, as well as field measurement from the National Oceanic and Atmospheric Administration (NOAA), will be used to test the accuracy of the developed solver, and simulation results will be compared to those of a solver based on the continuous Galerkin finite element method.

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Title: Calibrated Filtered Reduced Order Modeling

Author(s): Traian Iliescu, *Virginia Tech* ; *Xuping Xie, *Virginia Tech*.

We propose a calibrated filtered reduced order model (CF-ROM) framework for the numerical simulation of general nonlinear PDEs that are amenable to reduced order modeling. The novel CF-ROM framework consists of two steps: (i) In the first step, we use explicit ROM spatial filtering of the nonlinear PDE to construct a filtered ROM. This filtered ROM is low-dimensional, but is not closed (because of the nonlinearity in the given PDE). (ii) In the second step, we use a calibration procedure to close the filtered ROM, i.e., to model the interaction between the resolved and unresolved modes. To this end, we use a linear or quadratic ansatz to model this interaction and close the filtered ROM. To find the new coefficients in the closed filtered ROM, we solve an optimization problem that minimizes the difference between the full order model data and our ansatz. Although we use a fluid dynamics setting to illustrate how to construct and use the CF-ROM framework, we emphasize that it is built on general ideas of spatial filtering and optimization and is independent of (restrictive) phenomenological arguments. Thus, the CF-ROM framework can be applied to a wide variety of PDEs.

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Title: Approximation Algorithms for Big Data

Author(s): *Dongbin Xiu, *Ohio State University*.

One of the central tasks in scientific computing is to accurately approximate unknown target functions. This is typically done with the help of data — samples of the unknown functions. In statistics this falls into the realm of regression and machine learning. In mathematics, it is the central theme of approximation theory. The emergence of Big Data presents both opportunities and challenges. On one hand, big data introduces more information about the unknowns and, in principle, allows us to create more accurate models. On the other hand, data storage and processing become highly challenging. In this talk, we present a new framework for function approximation in the presence of big data. The new methods are of iterative nature and conduct approximation as data arrive sequentially. These sequential approximation methods require only vector operations and do not involve matrices. Moreover, they do not require the storage of the entire data sets. We present both the numerical algorithms, which are easy to implement, as well as rigorous analysis for their theoretical foundation.

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Title: Multi-Physics Coupled Computational Framework for Lithium-Ion Batteries under Mechanical Abusive Loading

Author(s): *Jun Xu, *Beihang University*; Binghe Liu, *Beihand University*.

Lithium-ion batteries (LIBs) are now widely applied to electric vehicles, such that the inevitable mechanical abuse safety problem during possible vehicle accidents has become a prominent barrier. This study first proposes a multi-physics computational framework model that couples mechanical, thermal, and electrochemical models to describe the complete process for a single LIB cell (i.e., from initial deformation, then final thermal runaway subject, to mechanical abusive loading). Experiments are also designed, which show the proposed model's suitable agreement with the established multi-physics model. Furthermore, parametric studies in terms of the governing factors, such as state of charge, loading speed, and deformation displacement are conducted and discussed. These studies reveal the underlying mechanism for the mechanical abuse safety of LIBs. This model can lay a solid foundation to understand LIB electrochemical and mechanical integrity, as well as provide critical guidance for battery safety designs.

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Title: Transitional Negative Stiffness as a New Form of Instability

Author(s): *Yuan Xu, Arcady Dyskin, Elena Pasternak, *Universityof Western Australia*.

A new mechanism of instability is proposed: a transitional negative stiffness. This is a momentary effect produced by developing fractures or broken bonds, which for a very short time of energy release act as a negative stiffness elements; after the fracture is formed it immediately turns into a conventional fracture with usual positive stiffness/compliance characteristics. We demonstrate that such fractures even in low concentrations are capable of momentarily bringing the Poisson's ratio of nearly incompressible material to 0.5. It is easy to demonstrate that elastic strictly incompressible material (Poisson's ratio equals 0.5) is unstable as it could support non-trivial wave-like displacement field even being free of loading. Such a non-trivial displacement field can lead to the observed strain localisation, post-peak softening and eventually the complete failure of the geomaterial. The existence of this mechanism is confirmed by discrete element modelling using PFC code.

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Title: Verification of Contact Stress in Elasticity Using a Surrogate Formulation

Author(s): *Zhaocheng Xuan, *Tianjin University of Tech&Edu*.

A method for verifying the contact stress of elastic bodies using a surrogate model is presented. The formulation of the total contact force, a fraction function with the numerator as a linear function and the denominator as a quadratic convex function, is first derived using the surrogate model of quadratic optimization for the contact problem. Then an upper bound formulation is obtained for the sum of the nodal contact forces, which is an explicit formulation of matrices of the finite element model, derived by maximizing the fraction function under the constraint that the sum of the normalized nodal contact forces is one. The bound is solved with the problem dimensions being only the number of contact nodes or node pairs, which are much smaller than the dimension for the original problem. Next, a scheme for constructing an upper bound on the contact stress is proposed that uses the bound on the sum of the nodal contact forces obtained on a fine finite element mesh and the nodal contact forces obtained on a coarse finite element mesh. Finally, the proposed method is verified through examples to demonstrate its feasibility and robustness.

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Title: Benchmark Results of a Mesh Moving Technique with Minimum-Height-Based Stiffening

Author(s): *Tomonori Yamada, Giwon Hong, Naoto Mitsume, Shinobu Yoshimura, *The University of Tokyo*.

This paper describes a mesh moving technique with minimum-height-based stiffening [1] for robust fluid-structure interaction (FSI) analysis with large deformation. The authors have been developing a general purpose parallel FSI analysis system [2] for large scale problems based on the line search partitioned approach [3] and applied to the analyses of flapping motion of MAV, fuel assemblies of the boiling water reactors and so on. The practical use of FSI analysis system requires the robustness for the parametric design of artifacts. Here, mesh moving technique is important for avoiding the failure of the analysis due to the mesh distortion. Hence, we propose a new mesh moving technique, minimum-height-based stiffening technique, where the mesh deformation of the fluid domain is virtually governed by the linear elastic equations and the stiffness of each element is determined according to its minimum height. The proposed technique is applied to two and three-dimensional benchmark problems and the performance is investigated. [1] T. Yamada, Y. Yamamoto, G. Hong, S. Yoshimura, A Mesh Moving Technique with Minimum-Height-Based Stiffening for Fluid-Structure Interaction Analysis, Mechanical Engineering Letters, 3, p.16-0657 (8 pages), 2017 [2] T. Yamada, G. Hong, S. Kataoka, S. Yoshimura, Parallel Partitioned Coupling Analysis System for Large-Scale Incompressible Viscous Fluid-structure Interaction Problems, Computers & Fluids, 141, pp.259-268, 2016. [3] T. Yamada, S. Yoshimura, Line Search Partitioned Approach for Fluid-Structure Interaction Analysis of Flapping Wing, Computer Modeling in Engineering and Sciences, 24-1, pp.51-60, 2008.

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Title: Method of Manufactured Solution for Large Deformation Finite Element Analysis of Hyperelasticity

Author(s): *Takahiro Yamada, *Yokohama National University*.

The method of manufactured solution proposed by Roache [1] is widely used to verify numerical codes in fluid dynamics. In this method, second derivatives of given solutions or spatial derivatives of stresses derived from given solutions are required to calculate body forces. However such derivatives can hardly be evaluated in nonlinear problems of solid materials and hence it has not been popular in solid mechanics. The author developed an alternative technique to calculate equivalent nodal vectors of body forces in the method of nearby problems [2] for finite element method. In this approach, calculation of the second order derivative of solutions can be avoided by utilizing the weak formulation of the problems of solid. The actual procedure to calculate equivalent nodal force vectors is similar to evaluation of internal force in the conventional nonlinear finite element procedures, in which the work product of the stress and virtual strain is integrated over the domain. We have applied our procedure to the problems of elasto-plasticity, which is a typical model of nonlinear materials. In this paper, we apply this approach to the method of manufactured solution for large deformation problems of hyperelasticty, which is often used to describe rubbler-like materials. In our approach, an arbitrary displacement field can be prescribed for manufactured solutions. However solids undergoing the large deformations usually exhibit incompressible or nearly incompressible behaviors and hence displacement fields of manufactured solutions are required to satisfy incompressibility or very small volumetric change. Thus we developed a procedure to construct displacement fields in which volumetric changes are controlled in the large deformation state. Several representative numerical results are presented to discuss the properties of proposed manufactured solutions. References: [1] P. J. Roache and S. Steinberg, “Symbolic manipulation and computational fluid dynamics,” AIAA Journal, Vol. 22, No. 10, 1984, pp. 1390–1394. [2] T. Yamada, "Verification Procedure Based on Method of Nearby Problems for Finite Element Analysis of Solid," ASME 2015 Verification and Validation symposium, 2015.

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Title: Shell Element to Represent Thickness-Stretch for Elastoplastic Problems

Author(s): *Takeki Yamamoto, *Tohoku University*; Takahiro Yamada, Kazumi Matsui, *Yokohama National University*.

In numerical simulations of sheet forming, the finite element method can be used to evaluate the plastic deformation of the blank. Continuum elements are capable of modeling the complex behavior of the sheet forming process. However, they lead to huge computational costs, which include pre-processing for mesh generation and solving a linear system of equations. On the other hand, structural elements, in which the plane stress condition in the transverse direction is imposed, are more efficient than continuum elements regarding computational costs. This assumption is only valid for thin structures, and hence structural elements can only be employed to predict simple bending behavior accurately when the thickness of the simulation model is small. Thus, conventional shell elements are not sufficient for simulating some situations involved in sheet forming, such as the change in thickness of the blank and the traction applied at the sheet-die interface. For the purpose of obtaining more accurate results by shell elements in such situations, it is necessary to develop a shell element in which thickness-stretch can be considered. This paper presents a quadrilateral shell element to represent thickness-stretch, and demonstrates its performance in large deformation analyses for elastoplastic materials. As a key technique of this study, additional degrees of freedom for evaluation of the thickness-stretch are introduced to the MITC4 shell element. The proposed shell element incorporates three features for the purpose of applying it to sheet forming simulations. One of them is the use of the three dimensional constitutive equation, and hence a plane stress state in the transverse direction is not assumed in this work. The second one is no numerical instabilities and artificial parameters. In the proposed formulation, neither the EAS formulation nor reduced integration technique is employed. The final feature is the avoidance of extreme increases in the degrees of freedom per element. Some numerical examples are presented to verify the capabilities of the proposed shell element in elastoplastic deformation problems.

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Title: Detailed Finite Element Analysis of E-Defense Shake Table Test of 10-Story Reinforced Concrete Building

Author(s): *Takuzo Yamashita, *NIED*; Tomoshi Miyamura, *Nihon University*; Makoto Ohsaki, *Kyoto University*.

E-Defense [1], NIED, possesses the world largest shaking table, which enables real scale buildings to be shaken against large earthquakes, such as the 1995 Hyogo-ken-Nambu earthquake. At NIED, numerical simulation code named E-Simulator [2], which aims to reproduce damage and collapse behavior of structures against large earthquakes, has been developed; data obtained from E-Defense shake table tests are used for its validation. In this study, numerical simulation of the E-Defense shake table test of the 10-story RC building is presented. Detailed model of the specimen is discretized by using solid element for concrete and truss element for steel rebar. Total number of DOFs amounts to 4,956,123. The number of solid elements and truss elements are 1,340,824 and 656,865, respectively. Concrete material is modeled by the extended Drucker-Prager law considering compressive failure and tensile crack and steel bar is modeled using the von-Mises yield criterion with isotropic hardening law. In order to solve large-scale dynamic nonlinear finite element problem, the coarse grid conjugate gradient method [3] (CGCG method) is employed as a linear solver. Time history response analysis is conducted for the model by inputting JMA Kobe seismic wave, which is seismic acceleration record observed during 1995 Hyogo-ken Nambu earthquake, at the bottom of base. As a result, maximum inter-story drift is observed at third story, which corresponds to the experimental result. Yielding process of the rebar inside the beam-to-column connection can be visualized, which is difficult to recognize from the experimental data. Simulation results are compared with a large amount of experimental measurement data so that accuracies of both local and global behaviors are evaluated. References: [1] Ohtani K., Ogawa N., Katayama T. and Shibata H.: Construction of E-Defense (3-D Full-Scale Earthquake Testing Facility). In: Proceedings of the 13th World Conference on Earthquake Engineering (13WCEE); Vancouver, Canada, Paper No. 189, August, 2004. [2] Yamashita T., Hori M. and Kajiwara K.: Petascale Computation for Earthquake Engineering, Computing in Science and Engineering, Vol.13, Issue 4, pp. 44-49, 2011. [3] Akiba H., Ohyama T. and Shibata Y.: CGCG Method for Structural Analysis and Its Enhancement■In: Proceedings of the 7th International Conference on Engineering Computational Technology (ECT2010), Valencia, Spain, 2010.

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Title: Weighted Reproducing Kernel Collocation Method for Solving Inverse Problems

Author(s): *Judy Yang, *National Chiao Tung University*; Pai-chen Guan, Chia-ming Fan, *National Taiwan Ocean University*.

A weighted reproducing kernel collocation method (weighted RKCM) is introduced to solve the inverse Cauchy problems governed by both homogeneous and inhomogeneous second-order linear partial differential equations. As the inverse Cauchy problem is known for its incomplete boundary conditions, how to efficiently obtain a numerical approximation with desired accuracy remains challenging. In this study, the main focuses are (1) The weighted RKCM for solving inverse Cauchy problems is shown to be formulated in the least-squares sense; (2) The error analysis is provided to show how the errors in the domain and on the boundary can be balanced with proper weights. As the locality of reproducing kernel approximation gets rid of the ill-conditioned system, it is shown that neither implementation of regularization nor implementation of iteration is needed to reach desired accuracy. The examples numerically demonstrate that the weighted RKCM improves the accuracy of solutions and exhibit optimal convergence rates in comparison with those obtained by the traditional direct collocation method.

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Title: Spectral Seismic Analysis of Underground Long Tunnels by 2.5D Finite/Infinite Element Approach

Author(s): *Yeong-Bin Yang, *National Taiwan University*; Hsiao-Hui Hung, *National Centre for Research on Earthquake Engineering*.

For a building constructed above the ground, it is conventional to assume that the building will be excited by an earthquake in the form of “ground” motion. Using the spectrum made available for a specific (design) earthquake, the modal superposition method can be adopted to calculate the base shear, as well as all the member forces, of the structure, considering the first several, separate natural frequencies. However, for an underground structure such as tunnels, it will be excited by an earthquake not via the ground motion, but by waves from all directions of the tunnel, due to reflections and refractions of the seismic waves generated by an underneath fault. Secondly, the frequencies that dominate the response of the tunnel are not separate or only a few. Theoretically, an “infinite number” of continuous frequencies of the surrounding soil body can affect the response of the tunnel. Thirdly, the boundary conditions of the above-ground structure are “finite” and well defined. But the tunnel is embedded in a half-space with infinite domain. All these factors make the seismic analysis of an underground tunnel difficult. To tackle this issue, a rational procedure is proposed for the seismic analysis of underground tunnels using recorded ground motions based on the 2.5D finite/infinite element approach. The near field and far field (with infinite domain) of the half space are modeled by finite and infinite elements, respectively. Using the 1D wave theory, the stress and displacement on the near-field boundary are computed for each spectral frequency of the earthquake. Then, equivalent seismic forces are computed for the near-field boundary for the earthquake spectrum. For long tunnels embedded in soils with uniform materials along the tunnel direction, the 2.5D approach can duly account for the wave transmission along the tunnel axis, which reduces to the 2D case for infinite wave velocity. The horizontal and vertical components of the 1999 Chi-Chi Earthquake (TCU068) are adopted as the free-field ground motions in the numerical analysis. The maximal stresses and distribution patterns of the tunnel section under the P- and SV-waves are thoroughly studied by the 2.5D and 2D approaches, which should prove useful to the design of underground tunnels. Reference Lin, K. C., Hung, H. H., Yang, J. P., and Yang, Y. B., Seismic analysis of underground tunnels by the 2.5D finite/infinite element approach, Soil Dyn. and Earthq. Eng., 85, 31-43, 2016.

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Title: DGDFT for Electronic Structure Calculation

Author(s): *Chao Yang, *Lawrence Berkeley National Lab*; Amartya Banerjee, Wei Hu, *Lawrence Berkeley National Laboratory*; Lin Lin, *UC Berkeley & Lawrence Berkeley National Laboratory*; John Pask, *Lawrence Livermore National Laboratory*.

We describe a massively parallel implementation of the recently developed discontinuous Galerkin density functional theory (DGDFT) method, for efficient large-scale Kohn-Sham DFT based electronic structure calculations. The DGDFT method uses adaptive local basis (ALB) functions generated on-the-fly during the self-consistent field (SCF) iteration to represent the solution to the Kohn-Sham equations. DGDFT can achieve 80% parallel efficiency on 128,000 high performance computing cores when it is used to study the electronic structure of 2D phosphorene systems with 3,500-14,000 atoms. We discuss a number of techniques employed in DGDFT to achieve high performance and accuracy, and show how DGDFT can be used to study properties of a variety of nanosystems.

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Title: A Computationally Efficient Process Modelling Approach for Selective Laser Melting

Author(s): *Yabin Yang, Can Ayas, *Delft University of Technology*.

Selective laser melting (SLM) is one of the main additive manufacturing methods suitable for metallic parts. Although SLM has nearly no limitation for geometrical complexity of the parts, undesired deformations and residual stresses are detrimental for the quality of the product. Appropriate process parameters and the scanning strategy need to be selected carefully to minimize deformations and residual stresses, but experimental trial and error is expensive and time consuming. Therefore, we present a computationally efficient thermo-mechanical model to investigate the influence of these parameters on the deformations and residual stresses of the SLM product. A semi-analytical thermal model is first established, in which an analytical solution for heat sources in semi-infinite space is utilised to capture the steep temperature gradient in the vicinity of the laser, and the boundary conditions are accounted for by finite element method (FEM). The temperature field is then used to calculate the thermal strain induced on the SLM product. To satisfy compatibility , corresponding elastic and plastic deformations and stresses are calculated using a temperature dependent elastic-plastic model with kinematic hardening rule. The melting behaviour is taken into account by setting the stress and strain to zero when the temperature is above the melting point. The mechanical analysis is assumed having little effect on the temperature field, thus the thermal and mechanical models are one way coupled. The proposed model is able to describe the development of temperature, associated deformation and stress-strain state within the product for any geometry during the SLM process. A multilayer-building-process for an overhanging structure is simulated using the proposed model. The residual stresses and part deformations are investigated as a function of different scanning strategies and the accuracy of the model is validated by experimental findings. The results prove that the scanning strategy is essential for the final shape of the product and hence should be accounted for in the process modelling.

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Title: Numerical Analysis of Plane Problems of Viscoelastic Functionally Gradient Material Based on a Temporally-Piecewise Adaptive Algorithm

Author(s): Linlin Zhang, Yiqian He, *Haitian Yang, Weian Yao, *Dalian Univ. Tech.*.

Functionally Gradient Material■FGM■has important applications in engineering areas, including shipbuilding industry, energy industry, artificial bionic and so on. In order to develop numerical methods for FGM to accurately calculate in both space and time domain, a new method is presented in this paper by combining a temporally-piecewise adaptive algorithm and FEM. By expanding variables by time domain expansion technique, the recursive scheme of the viscoelastic constitutive relation is obtained, and the viscoelasticity problem is transformed into a series of recursive spatial problems which are solved by FEM. Two numerical examples are given to verify and illustrate the proposed approach.

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Title: An Adaptive Discontinuous Galerkin Reduced-Basis Element Method for CFD

Author(s): *Masayuki Yano, *University of Toronto*.

We present an adaptive discontinuous Galerkin reduced basis element (DG-RBE) method for parametrized partial differential equations (PDEs) with applications in aerodynamics. The DG-RBE method leverages recent advances in discontinuous Galerkin methods and projection-based model reduction for parametrized PDEs. Specifically, the key ingredients of the method are the following: a DG method which provides stability for conservation laws and admits a flexible choice of approximation spaces; dual-weighted residual (DWR) error estimates and localization for quantities of interest; and a library of non-polynomial finite elements, called reduced basis elements (RBE), designed for specific solution features. The RBE library consists of spatially complex but parametrically simple features, such as boundary layers and trailing edge singularities. In the offline training stage, these reducible features and the associated tailored functions are identified by solving a number of representative training cases. In the online stage, the method, guided by a posteriori error estimates, incorporates an appropriate set of library functions to the approximation space for the specific problem. The DG-RBE formulation can be interpreted from two distinct perspectives. One one hand, the method extends the idea of output-based hp-adaptive finite element methods by exploiting non-polynomial approximation spaces, a perspective shared with generalized finite element methods. Thanks to the offline-trained library functions that are tailored specifically for the spatially rich but reducible features, the method requires a fewer degrees of freedom to achieve a given error tolerance than standard adaptive finite element methods. On the other hand, the DG-RBE method extends the envelope of projection-based model reduction to more general parametrized equations that exhibit a wide range of scales, nonlinearity, and limited stability as well as topological variations. In particular, the topological flexibility is provided by the fact that the RBE library is trained for reducible local features that may appear in many different cases, unlike in classical projection-based model reduction approaches that train the reduced model for a single specific case. This localized approach to model reduction greatly improves the flexibility of model reduction methods, an improvement needed to efficiently explore radically different designs. We demonstrate the DG-RBE method for parametrized Navier-Stokes equations associated with steady aerodynamic flows. We compare the approach with an output-based adaptive discontinuous Galerkin method.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: A Radial Basis Function Method on Problems of Blow-Ups in Nonlinear Parabolic Equations

Author(s): *Guangming Yao, *Clarkson University*.

A modified localized method of approximated particular solutions (LMAPS, also known as generalized RBF-FDM) is applied to investigate problems of blow-ups in nonlinear parabolic equations or system of such equations. Integrated (in radial space) polyharmonics spines RBFs and monotone iterations are used to overcome the difficulties of nonlinearity. The method requires neither domain nor boundary discretization and results in high accuracy and efficiency. For illustration, we are interested in the following questions through a couple of examples, starting from a smooth initial configuration: (1) does a blowup occur in finite time? (2) if so, where? (3) How fast does blow-up occur? (4) What are effects of the Dirichlet or Neumann boundary conditions?

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Boundary Integral Representation for Solenoidal Fields

Author(s): *Mykola Yasko, *Prof.*.

Many problems of the mathematical physics are described by the solenoidal vector fields. The boundary element (integral) method is a numerical method of solving the linear partial differential equations which have been formulated as integral equations. An integral representation of the desired functions is the basis for receiving the respective boundary integral equations. Method of weighted residuals is used for developing of the boundary integral representation for a solenoidal vector field. It is shown that the solenoidal vector in an arbitrary point of domain can be expressed as a series through its values and curls of the different order on the boundary domain. The boundary integral equations of the second kind for the solving of the boundary-valued problems are received for several linear problems: velocity of an incompressible irrotational flow new formulation for the Stokes flow linear Beltrami vector fields time-harmonic Maxwell equations It is marked that the given integral equations allow the effective numerical solving.

14th U.S. National Congress on Computational Mechanics
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Title: Weak Galerkin Method and Its Applications

Author(s): *Xiu Ye, *University of Arkansas at Litt*; Lin Mu, *Oak Ridge Nat'l Lab*; Junping Wang, *Natl Sci Found*.

Newly developed weak Galerkin (WG) finite element methods will be introduced for solving partial differential equations. The weak Galerkin method is a natural extension of the standard Galerkin finite element method for the function with discontinuity where classical derivatives are substituted by weakly defined derivatives. Therefore, the weak Galerkin methods have the flexibility of employing discontinuous elements and, at the same time, share the simple formulations of continuous finite element methods. The purpose of this presentation is to introduce the basis concept of the WG methods and to discuss the applications of the WG methods on fluid dynamics. A robust WG method will be presented for solving the Brinkman equations which converges uniformly. Also a simple WG method will be introduced to solve the Stokes equations in velocity pressure formulation in which both velocity and pressure are approximated by piecewise constant.

14th U.S. National Congress on Computational Mechanics
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Title: Ultrasound Imaging-Based Identification of Thermal Damage in Burnt Tissue

Author(s): *Hanglin Ye, *RensselaerPolytechnicInstitute*; Rahul, Saurabh Dargar, Suvranu De, *Rensselaer Polytechnic Institute*.

Burns are some of the most common injuries in both civilian and combat scenarios. Prompt and accurate identification of burn degree is of vital importance to the clinical treatment of burns since it helps reduce the mortality rate and shorten hospital stay of patients. However, the accuracy of clinical assessment of burn degree is only 50%-80% [1]. Hence, numerous experimental and numerical studies have been done to facilitate clinical determination of burn degree. Experimentally, various imaging techniques such as laser-Doppler imaging, videomicroscopy, and spatial frequency domain imaging have been developed to monitor burns. Computationally, bioheat transfer models combined with Arrhenius type damage model have been proposed to predict damage caused by thermal injuries. However most of these studies focus only on analyzing the results of burns, rather than studying the underlying physics and mechanism. As a result, there is scant information regarding changes in tissue properties, such as mechanical properties, resulting from burn injuries that are linked to altered tissue morphology [2]. We have developed an ultrasound elastography-based technique that is capable of characterizing burn injury by noninvasively measuring mechanical properties of skin and subcutaneous tissue. A robotic system, with integrated ultrasound imaging and force sensing capabilities [3], has been used to perform ex vivo compression tests on fresh porcine tissue samples. A reduced second order polynomial hyperelastic model has been used to characterize the mechanical response of the tissue. The mechanical properties of the tissue are obtained by iteratively solving a minimization problem: find the optimal mechanical parameters that minimize the difference between experimentally measured displacement as well as force fields and computationally predicted values in some norm. Our results suggest that while a linear tissue modulus is not a reliable indicator of tissue damage due to thermal injury, the nonlinear parameter of the hyperelastic model is capable of consistently detecting thermal damage of skin. References: [1] Hoeksema, H., et al. (2009) Burns 35: 36-45. [2] Ye, H., De, H. (2016) Burns DOI: 10.1016/j.burns.2016.11.014. [3] Dargar, S., Akyildiz, A., De, S. (2016) IEEE Trans. Biomed. Eng. DOI: 10.1109/TBME.2016.2644651.

14th U.S. National Congress on Computational Mechanics
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Title: Size-Dependent Deformation Behavior of Fluid-Filled Carbon Nanotubes under Electric Field

Author(s): *Hongfei Ye, *Dalian University of Technolog*; Lili Zhou, Junfei Zhao, Yonggang Zheng, Hongwu Zhang, Zhen Chen, *Dalian University of Technology*.

Carbon nanotubes (CNTs) are ideal candidates for structural elements or functional components in nanoscale systems. Controlling the deformation of CNTs through external fields has great potential applications in micro-electro-mechanical systems, microfluidic chips, etc. In this study, the deformation behaviors of pure water and salt water-filled CNTs under the electric field are investigated by using molecular dynamics (MD) simulations and classical mechanical theory. Here, six types of CNTs ((6, 6), (8, 8), (10, 10), (12, 12), (16, 16) and (20, 20) CNTs) are considered in order to examine size dependence of the deformation behavior of fluid-filled CNTs. The simulation results reveal that the pure water-filled CNTs will be bent under the electric field with orthogonal components. For the same CNTs, the electric field-induced bending deflection increases with the increase in the electric field intensity. However, the bending deflection exhibits a nonlinear dependence on the diameter of the CNTs. As for the salt water-filled CNTs, the bending deflection is more obvious due to the introduction of the ions. Moreover, the theoretical model is also constructed to describe the deformation behavior of the fluid-filled CNTs, which is founded on the basis of the bending moment of water molecules near the CNT wall and the electric force of the ions. The present research reveals the controllable performance of fluid-filled CNTs and provides theoretical guidance and reference for the experimental works. By means of the controllable deformation of fluid-filled CNTs, the present investigation also opens up a new avenue in the design and fabrication of nanoscale controlling units, high-sensitive sensors, etc. The supports from the National Natural Science Foundation of China (11672063, 11302037, 91315302 and 11472117), the 111 Project (B08014) and Fundamental Research Funds for the Central Universities are gratefully acknowledged.

14th U.S. National Congress on Computational Mechanics
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Title: Mesh Dependency Performance of Nonlinear Solid Analysis Using Isogeometric Elements

Author(s): *Yuta Yokoyama, Shigenobu Okazawa, *University of Yamanashi*.

Isogeometric analysis has recently become very popular for numerical modeling of structures and fluids. Basis functions generated from NURBS (Non-Uniform Rational B-Spline) are employed to construct an exact geometric model obtained from CAD. In this paper, we perform mesh dependency performance of isogeometric elements in nonlinear solid analysis.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Modeling Interfacial Behavior of Responsive Polyelectrolyte-Grafted Nanoparticles

Author(s): Shiyi Qin, *Xin Yong, *Binghamton University*.

We use dissipative particle dynamics (DPD) to discover the interfacial adsorption and self-assembly of pH-responsive polyelectrolyte-grafted nanoparticles (PNP) in a water-oil binary system. The electrostatic interactions between charged beads in the presence of dielectric discontinuity are modeled by exploiting a modified particle-mesh method, which applies an iterative Poisson solver on a uniform grid. The degree of ionization of PNP at a given pH is determined by the degree of ionization of grafted polyelectrolytes through the Henderson-Hasselbalch relation. We simulate the adsorption behavior of a single PNP from the aqueous phase. Through changing the degree of ionization, we explore the influence of pH on the adsorption behavior and show that the electrostatic interactions significantly modulate the adsorption. Contact angle at the interface, morphology of PNP, and pair correlation function between oil and particle are probed to characterize the adsorption behavior. Furthermore, the self-assembly of multiple PNPs at the water-oil interface is studied. The surface coverages and detailed structure of the PNP layer under the influence of pH are quantified.

14th U.S. National Congress on Computational Mechanics
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Title: New Particle Difference Algorithm for Material Nonlinear Problem

Author(s): *Young-Cheol Yoon, *Myongji College*; Jeong-Hoon Song, *University of Colorado Boulder*.

This study presents a novel particle difference algorithm for material nonlinearity problem. The Particle Difference Method (PDM) constructs strong formulation employing the fast derivative approximation and discretizes governing partial differential equations based on a node-wise manner. However, the conventional PDM is not able to explicitly handle constitutive equations since it usually solves solid mechanics problems by using the Navier's equation that unifies unknowns into displacement. In this study, a double derivative approximation is proposed to treat the constitutive equation of nonlinear material in the framework of strong formulation; it utilizes the first order particle derivative approximation two times to treat the second order PDE. Thus, the equilibrium equation can be directly linearized by the Newton method and an iterative procedure is applied to get a convergent solution. Stresses and internal variables are updated by the return mapping algorithm and the use of algorithmic tangent modulus improves effectiveness of the nonlinear procedure. The consistency of the double derivative approximation is shown by performing the reproducing property test. Also, accuracy of the developed procedure is verified by solving several benchmark problems involving nonlinear material.

14th U.S. National Congress on Computational Mechanics
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Title: Analysis of Flapping Motion Considering Kinematic Optimization by Partitioned Iterative FSI Analysis System

Author(s): Giwon Hong, Tomonori Yamada, Naoto Mitsume, *Shinobu Yoshimura, *The University of Tokyo*.

Most of flying animals such as insects and birds fly by utilizing flapping wings. Under the inspiration of them, the mechanisms of flapping flight and its application have been studied in experimental biology and mechanics. Especially, flapping-wing micro air vehicles (MAVs) have been developed with the purpose of environmental monitoring or searching in hazardous areas. The MAVs are expected to demonstrate efficient aerodynamic performance at low Reynolds numbers compared with ones using fixed wings or rotary wings [1]. It is still challenging to design maneuverable flapping-wing MAVs because there are still unclear factors on flapping flight. Unsteady and complex motions of an flapping wing disturb the understanding of the flight by actual observation. Therefore, by using a fluid-structure interaction (FSI) analysis, we have researched to analyze various flapping motions and to attain the knowledge of an optimized wing in morphology and kinematics. In this research, we focus on designing kinematic models to improve flapping aerodynamic performance by utilizing three kinematic mechanisms, i.e. flapping, pitching and lead-lag. The flapping motions are analyzed by using the three-dimensional FSI analysis system employing partitioned iterative coupling methods [2], which allow us to utilize existing solvers: a parallel FEM flow solver FrontFlow/blue and a parallel FEM structure solver ADVENTURE_Solid. For improving the stability of the system, we examine iterative methods and mesh-control techniques [3] to deal with massive mesh moving. Finally, we evaluate the result of parametric studies to design optimized kinematic models and the improvement of the FSI analysis system. REFERENCES [1] M.H. Dickinson, F.O. Lehmann, S.P. Sane, Wing rotation and the aerodynamic basis of insect flight, Science, Vol. 284, pp.1954–1960, 1999 [2] T. Yamada, G. Hong, S. Kataoka, S. Yoshimura, A parallel iterative partitioned coupling analysis system for large-scale incompressible viscous flow-structure interaction problems, Computers & Fluids, Vol. 141, pp.259–268, 2016 [3] T. Yamada, Y. Yamamoto, G. Hong, S. Yoshimura, A mesh moving technique with minimum-height-based stiffening for fluid-structure interaction analysis, Mechanical Engineering Letters, Vol. 3, p.16-00657 (8 pages), 2016

14th U.S. National Congress on Computational Mechanics
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Title: A Generalized Mimetic Finite Difference Method and Two-Point Flux Schemes over Voronoi Diagrams

Author(s): *Ivan Yotov, *University of Pittsburgh*; Omar Al-Hinai, *Siemens PLM*; Mary Wheeler, *The University of Texas at Austin*.

We present a generalization of the mimetic finite difference method for second order elliptic problems that extends the family of convergent schemes to include two-point flux approximation (TPFA) methods over general Voronoi meshes, which are known to satisfy the discrete maximum principle. The method satisfies a modified consistency condition, which utilizes element and face weighting functions. This results in shifting the points on the elements and faces where the pressure and the flux are most accurately approximated. The flux bilinear form is non-symmetric in general, although it reduces to a symmetric form in the case of TPFA. It can be defined as the L2-inner product of vectors in two H-div discrete spaces, which are constructed via suitable lifting operators. The method can be viewed as a H-div conforming Petrov-Galerkin mixed finite element method. We prove first-order convergence in pressure and flux, and superconvergence of the pressure under further restrictions. Numerical results are presented to support the theory and illustrate the performance of the method.

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Title: Higher-Order Multi-Dimensional Limiting Strategy for Subcell Resolution in Unstructured Triangular Meshes

Author(s): *Hojun You, Chongam Kim, *Seoul National University*.

Unstructured grid-based higher-order methods are emerging as the latest trend in computational fluid dynamics (CFD) community due to its advantages such as grid flexibility, high scalability and better capability to get high-order accurate solutions with affordable computational cost. However, it still faces a number of issues to resolve. Among them, inventing a robust and accurate shock-capturing method providing higher-order subcell resolution is a very challenging issue. The present work deals with a new improvement of hierarchical multi-dimensional limiting process (hMLP) for providing reliable and robust higher-order subcell distributions within the framework of discontinuous Galerkin (DG) method and flux reconstruction/correction procedure via reconstruction (FR/CPR) method under unstructured triangular meshes. MLP limiting had been originally developed within the framework of finite volume method (FVM) by applying the MLP condition to its neighboring vertices that can be extremum when assuming linear approximation. This limiting mechanism is mathematically supported by the local maximum principle that guarantees multi-dimensional monotonicity. From previous studies, MLP was successfully extended to higher-order methods such as DG and FR/CPR methods in a hierarchical manner. Hierarchical MLP (hMLP) employs an extended version of the MLP condition called the P1-projected MLP condition to capture troubled-cells. After marking troubled-cells, smooth extrema detector is then introduced to preserve required accuracy across smooth extrema. From extensive computations, it was observed that hMLP yields outstanding performances such as preserving the formal order of accuracy in smooth region and maintaining solution monotonicity in the sense of cell-averaged value around discontinuities. At the same time, however, it was observed that spurious subcell Gibbs oscillations still exist near discontinuities in higher-order subcell distribution. In order to eliminate subcell Gibbs oscillations, a criterion called the MLP boundary detector is newly introduced. It is designed by quantifying and scaling the solution jump across a cell boundary-edge to identify whether the boundary-edge belongs to a troubled-cell. Subcell Gibbs oscillations can be efficiently controlled by identifying the number of troubled-boundary of a target cell. The resulting hMLP combined with the MLP boundary detector, hMLP_BD, provides quite desirable performances in triangular meshes. It not only maintains the advantages of the hMLP limiting but also provides reliable and robust higher-order subcell distributions by efficiently removing subcell Gibbs oscillations.

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Title: High Order Diffuse Domain Methods for Partial Differential Equations with Dirichlet Boundary Conditions in Complex Geometries

Author(s): *Fei Yu, John Lowengrub, *UC Irvine*.

Previously, Li et al. (Comm. Math. Sci., 7:81-107, 2009) developed a diffuse domain method (DDM) in order to solve partial differential equations (PDE) in complex geometries. In this approach the complex geometry was embedded into a larger, regular domain. The original PDE was reformulated with a phase field function, which smoothly approximates the characteristic function of the original domain, plus additional source terms that approximate the boundary conditions. Later Lervåg and Lowengrub (Comm. Math. Sci., 2014) performed a matched asymptotic analysis of general diffuse domain methods for Neumann and Robin boundary conditions and showed that for certain choices of boundary condition approximations the DDM is second-order accurate in epsilon, which characterizes the width of the region over which the characteristic function is smoothed. We extend this analysis to PDEs with Dirichlet boundary conditions and show that by perturbing the reformulated equation in a certain way, we are able to achieve second-order accuracy in epsilon. Our analytic results are confirmed numerically in both the L^2 and L^∞ norm for selected test cases.

14th U.S. National Congress on Computational Mechanics
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Title: Aeroacoustic Simulation of Nearly Incompressible Flow Coupled with Deformable Solid

Author(s): *Feimi Yu, Lucy Zhang, *Rensselaer Polytechnic Inst.*.

The evaluation of the aeroacoustic perturbation with low Mach number in fluid-structure interactions is challenging. In this talk, we will introduce an aeroacoustic model for nearly incompressible isentropic flows, which is then incorporated into a fluid-structure interaction framework to evaluate the impact of pressure fluctuation on a deformable solid. The pressure fluctuations caused by compression of the fluid in a subsonic flow (typically 10e-2 Pa) has large disparities in the magnitudes with the atmospheric pressure, making it difficult to capture the acoustic properties correctly and invalid to assume full incompressibility in a flow. The proposed aeroacoustic model captures the fluctuation in pressure field due to the compression of the fluid wave during an acoustic wave generation and propagation process without the inclusion of a fully compressible representation of the fluid or super-imposed linear models of pressure perturbation. This model is successfully coupled into a fluid-structure interaction framework to evaluate the compressibility effects in a fully-coupled fluid-structure interactions. A detailed study of flow past a deformable leaflet shows that sinusoidal pressure perturbations yields a larger amplitude of oscillation with the inclusion of slight compressibility comparing to that of with full incompressibility. This approach is then applied to the study of vocal fold vibrations where a sustained vibration is obtained utilizing the fully coupled aeroelasticity and the proposed aeroacoustic model.

14th U.S. National Congress on Computational Mechanics
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Title: Finite Element Modeling Approach for Protein Dynamics

Author(s): *Giseok Yun, Jaehoon Kim, Jae-Young Lee, Do-Nyun Kim, *Seoul National University*.

Analysis of protein dynamics is important to understand its link to biological functions. Classical atomistic methods such as molecular dynamics simulation have been widely used to investigate the protein dynamics in detail, but they are usually limited by the time and length scales that can be simulated. Finite element modeling approach can be employed instead, and has demonstrated its capability to explore the slow, collective motion of proteins efficiently. Here, we present our recent effort to further develop the finite element modeling approach for protein dynamics including model generation, parameter sensitivity, and incorporating solvent damping into the model. Comparison with experimentally measured properties will be also provided. References: [1] D.-N. Kim, C.-T. Nguyen, and M. Bathe, Conformational dynamics of supramolecular protein assemblies, Journal of Structural Biology, 173(2011), 261-270. [2] D.-N. Kim, J. Altschuler, C. Strong, G. McGill, and M. Bathe, Conformational dynamics data bank: a database for conformational dynamics of proteins and supramolecular protein assemblies, Nucleic Acids Research, 39(2011), 451-455. [3] J. Kim, J.-G. Kim, G. Yun, P.-S. Lee, and D.-N. Kim, Toward modular analysis of supramolecular protein assemblies, Journal of Chemical Theory and Computation, 11(2015), 4260-4272. Acknowledgements: This research was supported by the EDucation-research Integration through Simulation On the Net (EDISON) Program (Grant No. 2014M3C1A6038842), the Global Frontier R&D Program on Center for Wave Energy Control based on Metamaterials (Grant No. 2014M3A6B3063711), and the Basic Science Research Program (Grant No. 2016R1C1B2011098) through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future Planning.

14th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Viscoelastic Damping Layers for Transient Vibration Reduction of Shell Structures

Author(s): *Kyeong-Soo Yun, Sung-Kie Youn, *KAIST*.

Viscoelastic damping layers are often attached to the shell structures for reducing the structural dynamic responses. However, a full-coverage damping layer treatment is not practical, since it may add excessive weight to the base shell structures. Therefore, it is highly desired to optimize the viscoelastic layer for effectively suppressing the dynamic responses. This design problem may be formulated as topology optimization problem. The dynamic responses are calculated with the Newmark method in time domain. Also, performance indices are introduced to measure the dynamic responses. The design objective is to minimize the performance indices by distributing a given amount of viscoelastic materials. A sensitivity analysis procedure is developed based on the adjoint variable method. The discretize-then-differentiate approach is adopted to calculate the consistent sensitivity. Several numerical examples with different types of objective functions are presented. The proposed method is validated by comparing the optimized results with those of the uniformly distributed structures. The influences of the performance indices are also discussed.

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Title: Parallel Elastic-Plastic Analysis Using a Domain Decomposition Method with a Nonlinear Solver

Author(s): *Yasunori Yusa, Hiroshi Okada, *Tokyo University of Science*; Tomonori Yamada, Shinobu Yoshimura, *The University of Tokyo*.

To assess the integrity of real large-scale structures, elastic-plastic finite element analysis can be helpful. To analyze large-scale structures, parallel finite element method based on domain decomposition method is used. In domain decomposition method, the analysis model is decomposed into multiple subdomains for parallel processing. The system of equations about the subdomain interface degrees of freedom (DOFs) is to be solved by an iterative solver. At every iteration step of the iterative solver, each subdomain is analyzed under assumed boundary conditions on the subdomain interface. When the system of equations about the interface DOFs is linear, it is frequently solved by preconditioned conjugate gradient (PCG) method. However, when it is nonlinear, it should be solved by a nonlinear solution method. In nonlinear problems, such as an elastic-plastic problem, the Newton-Raphson method is commonly used. The Newton-Raphson method needs to solve a linear system of equations at every iteration step. Therefore, a domain decomposition method with Newton-Raphson method requires a double-loop algorithm whose outer loop is Newton-Raphson iteration and whose inner loop is PCG iteration. However, this double-loop algorithm may be wasteful in the sense of its computational cost. Then, in this study, to solve the nonlinear system of equations about the interface DOFs, fixed-point iteration method and quasi-Newton method is applied. These methods do not require the double-loop algorithm. In the presentation, an elastic-plastic problem is analyzed by domain decomposition method that is based on Newton-Raphson method as well as the other nonlinear solution methods. The convergence performance is carefully investigated.

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Title: Modeling Ni/Al High Energy Ball Milled Composites Using the Sharp Volumetric Billboard Method

Author(s): *Dewen Yushu, Sangmin Lee, Karel Matouš, *University of Notre Dame*.

Predicting behavior of heterogeneous materials through numerical modeling is a challenging topic due to the extremely high computational cost required to resolve all of the geometrical complexities. To address this problem, various homogenization models have been developed to predict the mechanical behavior of materials. However, accurately predicting highly nonlinear material response with prominent localized behavior remains elusive. The focus of this work is to predict the macro- and micro-mechanical behavior of high energy ball milled (HEBM) Ni/Al composites through sharp volumetric billboard (SVB) based modeling. This SVB based modeling stems from the volumetric billboard (VB) method, a Google Earth like multi-resolution modeling strategy in computer graphics. This technique is a data-compression strategy developed for real time 3D image rendering. By creating VB series of an object, the data amount is greatly decreased while object shape is visually retained. In our work, we analyze the statistical and physical implications of the VB technique, and enhance it through the SVB scheme. A sharpening filter is created to reconstruct the original material contrast on coarser microstructures. We propose a contrast-based minimization problem and a corresponding numerical algorithm that approximates the minima through a fast sweeping strategy with local volume preservation. In our work, we focus on reactive composites produced by High Energy Ball Milling (HEBM), a promising strategy to control the initial degree and character of the inter-mixing between various components. We utilize a fine scale microstructure from microtomography, and create levels of detail (LODs) from the SVB scheme. The first and second order probability functions are computed, and both exhibit consistency after large data reduction (1/8 the amount of finer SVB). Then, we use a parallel generalized nite element code, PGFem3D, to compute the mechanical behavior under a tension-relaxation loading pro file using crystal plasticity constitutive equations. Two sets of simulations are performed. Firstly, we adopt identical texture to avoid potential side-effects from the crystal orientation mapping among LODs. Secondly, random texture is adopted to simulate the real material texture. The macro- and micro-mechanical robustness of data compression is demonstrated through corresponding error analysis.

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Title: Phase Field Modeling of Hydraulic Fracturing with Interfacial Damage in Highly Heterogeneous Fluid-Saturated Porous Media

Author(s): *Julien Yvonnet, Liang Xia, *Université Paris-Est*; Siavash Ghabezloo, *Ecole des Ponts Paris Tech*.

In this work, we propose a numerical framework for modeling hydraulic fracturing or cracking in fluid-saturated porous media, taking into account: (a) the presence of heterogeneities; (b) interfacial damage between the inclusions and the matrix; (c) fluid flow within both matrix and interface cracks; (d) the possibility to define the geometry of the heterogeneous media in the form of regular grids of voxels e.g. as obtained from experimental imaging techniques. The developed numerical framework is based on the phase field method with a regularized description of both bulk and interface discontinuities, extended to a fully coupled hydro-mechanical framework. Both 2D and 3D examples are presented for hydro-mechanical microcracking initiation and propagation in voxel-based models of complex heterogeneous media with interfacial damage between the inclusions and the matrix.

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Title: Realistic Crack Patterns Obtained Using an Approach Coupling Finite Element Method and Peridynamics

Author(s): *Mirco Zaccariotto, Davide Tomasi, *University of Padova (Italy)*; Ugo Galvanetto, *University pf Padova (Italy)*.

The pervasive presence of cracks in many structures, in particular in aerospace engineering, still represents a challenge for the engineer who wants to simulate the full structural life cycle. The presence of cracks in a solid represents a discontinuity in the displacement field, in this case the hypothesis of the continuity of the domain required by Classical Continuum Mechanics (CCM) is not satisfied. Many scientists have tried to equip CCM based methods, in particular the Finite Element Method (FEM), with the capability to simulate crack propagation: X-Fem, element erosion, interface-elements with CZM, phase field theory are probably the most popular approaches, but all of them have some drawbacks [1]. Peridynamics (PD) is a continuum theory based on a non-local approach and formulated with integral equations [2]. This theory is particularly suitable for dealing with crack propagation in solid materials since it does not assume continuous displacements. However PD is not computationally efficient, due to the non-local nature of the approach. Therefore, it would be very convenient to apply the PD based computational method only to the parts of the problem domain where phenomena such as damage and fracture strongly influence the solution, whereas the remaining part would be modelled with the more efficient FEM. In particular FEM would be used at the boundaries to avoid the soft boundary effect typical of PD. Such an approach requires an effective coupling, between the two parts of the model, that should not introduce inaccuracies such as ghost forces or spurious displacement components. The present work introduces a new coupling technique which constitutes a significant step forward with respect to that presented in [3]. In reference [3] the PD grid and the FEM mesh had to be characterised by the same spacing. The present approach overcomes such a restriction so that it makes possible to couple a fine PD grid with a coarser FEM mesh and in this way improves considerably the computational efficiency of the overall computational method. The new numerical technique is applied to static and dynamic problems in 1, 2 and 3-D with any type of crack pattern. In this way a new computational tool is produced which provides the standard FEM with the capability to effectively and efficiently study 3D problems with crack propagation phenomena. References [1] F. Bobaru, J. T. Foster, P. H. Geubelle, S. A. Silling, Handbook of Peridynamic Modeling, CRC Press, (2016). [2] S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. J Mech Physic Solids, 48(1), 175-209, (2000). [3] U. Galvanetto, T. Mudric, A. Shojaei, M. Zaccariotto, An effective way to couple FEM meshes and Peridynamics grids for the solution of static equilibrium problems, Mech Res Comm 76, 41–47, (2016).

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July 17-20, 2017, Montreal, Quebec, Canada

Title: Gradient-Based Methods for Detecting the Effective Dimension of Nonlinear Bayesian Inverse Problems

Author(s): *Olivier Zahm, Youssef Marzouk, *MIT*; Tiangang Cui, *Monash University*; Kody Law, *Oak Ridge National Lab*.

A large-scale Bayesian inverse problem has a low effective dimension when the data are informative only on a low-dimensional subspace of the input parameter space. Detecting this subspace is essential for reducing the complexity of the inverse problem. For example, this subspace can be used to improve the performance of MCMC algorithms and to facilitate the construction of surrogates for expensive likelihood functions. Several different methods have recently been proposed to construct such a subspace---in particular, gradient-based approaches like the likelihood-informed subspace (LIS) method and the active subspace (AS) method. In the context of nonlinear inverse problems, however, both methods are essentially heuristics whose approximation properties, relative to an optimal approximation, are poorly understood. We introduce a best approximation problem for the posterior distribution, which defines the best possible parameter space decomposition. Solving this problem in general non-Gaussian/non-linear cases, however, appears intractable. Instead, we develop a new bound on the Kullback-Leibler divergence between the posterior distribution and the approximation induced by a parameter space decomposition. We then identify the subspace that minimizes this bound, and compute it using gradients of the likelihood function. This approach allows the approximation error to be rigorously controlled. We also address the question of efficient computation of the parameter space decomposition in case only a limited number of gradient evaluations are allowed. A numerical comparison with existing methods favorably illustrates the performance of our new method.

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Title: Adjoint-Based Optimization of Time-Dependent Fluid-Structure Systems Using a High-Order Discontinuous Galerkin Discretization

Author(s): *Matthew Zahr, *LBNL, UC Berkeley*; Per-Olof Persson, *UC Berkeley, LBNL*.

The design and control of engineering and scientific systems often calls for the optimization of a system that depends on the interaction between fluid flow and structural deformation. For example, the design and control of Micro Aerial Vehicles (MAVs) is heavily dependent on the interaction between the light, flexible wings and the surrounding fluid. An optimal design that leads to a lightweight MAV and energetically optimal flapping motion can only be realized if the interaction between the fluid and structure is considered. In this work we develop the fully discrete adjoint equations and corresponding adjoint method for a high-order discretization of Fluid-Structure Interaction (FSI). Following the work in [1, 2], a system of conservation laws are transformed to a fixed reference domain using an Arbitrary Lagrangian Eulerian formulation and discretized using a high-order discontinuous Galerkin method. The structural equations are discretized using the continuous Galerkin finite element method. The primary innovation is the use of a high-order implicit-explicit Runge-Kutta scheme for temporal discretization of the monolithic fluid-structure system that ensures both the fluid and structural solvers can be re-used without need for a specialized monolithic solver. The fully discrete adjoint equations preserve this property and, therefore, do not constitute a major implementation effort given the primal implementation. The adjoint method is used in this work to compute gradients of quantities of interest that comprise the objective and constraint func- tions of relevant FSI model problems related to energetically optimal flapping flight and energy harvesting.

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Title: Parametric Simulations of Trileaflet Valve Function

Author(s): *Rana Zakerzadeh, *University of Texas at Austin*; Ming-Chen Hsu, *Department of Mechanical Engineering, Iowa State University*; Michael Sacks, *Institute for Computational Engineering and Science, Department of Biomedical Engineering, The University of Texas at Austin*.

In this work, we discuss a computational framework for modeling the dynamics of a trileaflet heart valve using a fluid-structure interaction approach to identify what makes the heart valve to function properly. More precisely, a parametric study is carried out to identify the role of leaflet's shape and material model on valve performance, indicated by the effective orifice area during the opening and the coaptation area during the closing as well as the stress/strain field. The results of this study can provide guidelines for detecting anomalies in the natural valve or improving leaflet tissue's design in the artificial valves to enhance valve durability. A Rhino-Grasshopper based interactive geometry design platform is used to construct the valve according to the aortic root geometry. leaflets are modeled as a thin shell structure using different constitutive models. In particular, both nonlinear isotropic and anisotropic material models have been considered and compared. We simulate the valve deformations with various perturbations of the tissue properties including the collagenous fiber direction, as well as the fiber and matrix stiffness to investigate the effect of alteration of the tissue mechanical properties. We also examine the effect of changing leaflet's shape on valve dynamics with the parameterization of the leaflet geometry, which allows for generating various perturbations of the leaflet design by adjusting some geometrical parameters such as leaflet's thickness and surface curvature. To approximate this problem, we used an immersogeometric fluid-structure interaction (FSI) methodology. We simulate the coupling of the deforming aortic root, heart valves, and the surrounding blood flow under physiological conditions through several cardiac cycles. Due to the complex motion of the heart valve leaflets, the blood flow domain undergoes large deformations, including changes of topology. The FSI simulations are carried out using our hybrid immersogeometric/arbitrary Lagrangian–Eulerian methodology, which allows us to efficiently perform a computation that combines a boundary-fitted, deforming-mesh treatment of the artery with a non-boundary-fitted treatment of the leaflets. The attachment edge of the leaflet is coupled with the arterial wall motion using a penalty formulation. Using the results of our parametric study, we obtain the acceptable ranges for our design criteria and highlight the potentially dangerous stress/strain concentrations. We observed a noticeable influence of the leaflet geometry and the material properties of the valve on the effective orifice area and the overall tissue deformation respectively. The results demonstrate the effectiveness of the proposed platform with greater levels of physical realism.

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Title: A Three-Dimensional DEM-FEM Modeling of Pneumatic Tire-Sand Soil Interaction

Author(s): *Mengyan Zang, *South China University of Tech*; Zumei Zheng, *South China University of Technology*.

This work is concerned with a three-dimensional DEM-FEM modeling of pneumatic tire-sand soil interactions. The pneumatic tire is meshed into linear hexahedral finite elements and the sand soil is modeled by the multi-sphere discrete elements. A contact detection algorithm is obligated to the interface between the pneumatic tire and the sand soil. Here, the multi-sphere discrete elements are generated by overlapping several spheres in the same size and used to characterize the three-dimensional particle shape of the sand soil. A numerical analysis code is implemented into the in-house developed code and travel performance of the pneumatic tire is investigated, where travel parameters such as gross tractive, drawbar pull, running resistance and sinkage of the pneumatic tires with different tread patterns (smooth and block) are obtained. There is a good agreement between the simulations and the experimental results, which demonstrate the effectiveness of the proposed DEM-FEM model.

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Title: Smart Ferro Fluid for Shock Absorber Main Landing Gear

Author(s): *Abolghasem Zare shahneh, *Cranfield University*.

A computational approach to alternate of smart fluids such as Ferro fluids, Electro Rheological fluids and Magneto Rheological fluids and its applications to design active controlled devices motivates the aerospace designers to adapt this technology to the aerospace applications. Especially implementing the smart fluid technology in the field of landing gear shock absorber improves landing gear shock absorber performance. This paper shows the outcome of the design of a landing gear shock absorber hydraulic system using Magneto Rheological and investigates its potential to generate variable damping force. Landing gear shock absorber hydraulic system compatible to use with Magneto Rheological fluid is designed and its performance under dynamic piston velocity is analyzed. The analysis results demonstrated that the Magneto Rheological fluid is capable of generating variable damping force at different magnetic flux densities for constant orifice area. The damping force generated by the Magneto Rheological fluid shock absorber in the absence of the magnetic field is about 4300 kg and same shock absorber with conventional oil can generate the damping force of 4450 kg for same orifice area and piston telescopic velocity. It shows that Magneto Rheological shock absorber is equal to the conventional shock absorber in the absence of the applied fields. The designed Magneto Rheological fluid shock absorber with the applied magnetic field can generate the damping force in the range of 1850 kg to 10464 kg for an applied magnetic field densities of 0.1 T to 0.9 T. This result lays a way for landing gear designers to design an adaptive landing gear by integrating a control system to it.

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Title: New Methods for Grid-shell Form-Finding

Author(s): *Tomas Zegard, *PUC Chile*; Yang Jiang, Glaucio Paulino, *Georgia Tech*; William Baker, *SOM LLP*.

The problem of designing a grid-shell for (close to) optimal performance is one of geometry. Various methods for this purpose have been proposed through history, both analytical and experimental. This presentation addresses two form finding methods for grid-shells: one method follows the idea behind old form-finding experiments considering strings in a large deformation setting; while the second method is based on an augmented version of the ground structure (topology optimization) method. Design-dependent loads are considered in both cases. Therefore, the algorithms iterate towards a converged solution. The proposed methods are compared to the (well-known) force density method, with their advantages and drawbacks compared and highlighted.

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Title: Combining ALE Flow Computations and Embedded Boundary Methods for Multi-Physics Problems

Author(s): *Xianyi Zeng, *University of Texas at El Paso*; Kangan Li, Guglielmo Scovazzi, *Duke University*.

Conventional strategies to handle multi-physics problems with flows include body-fitted methods and embedded boundary methods. The former is suitable when the material interface has small or moderate displacements and deformations; and a core component of such methods is an arbitrary Lagrangian-Eulerian (ALE) flow solver. However, when the material interface undergoes large deformation or even topological changes, embedded boundary methods (EBM) often perform better than body-fitted schemes. Constructing an embedded boundary method in the ALE fluid framework is thusly able to handle problems involve both scenarios. For example, in the simulation of liquid-gas-solid interactions, it will be advantageous to couple the solid with the liquid/gas mixture using an ALE framework, whereas treat the interface between the liquid and the gas by an embedded material interface. In this work, we make an attempt in this direction by proposing a ghost fluid method for a monolithic ALE flow solver for shock hydrodynamics. Particularly, the ALE flow solver [1] discretizes the Euler equation using nodal elements; it is characterized by a variational multiscale (VMS) stabilization and an entropy viscosity [2] to capture shocks. The interface between different fluids is handled by a ghost fluid method, where ghost values are populated for each fluid phase to enforce the transmission condition at the material interface. The ghost values are constructed by solving a local multi-material Riemann problem, in order to capture the correct physics when strong discontinuities occur. From one time step to the next, the ALE flow solver is used to update the flow variables for each single material at both the real fluid nodes and a few layers of ghost fluid nodes; the latter are the candidates that may be swept by the moving interface and undergo phase change. Finally, we couple the ALE-EBM flow solver with a stabilized finite element for transient solid dynamics [3] to compute the interaction among nearly incompressible viscoelastic structures, slightly compressible liquids, and compressible gases. References: [1] Xianyi Zeng, Guglielmo Scovazzi, "A variational multiscale finite element method for monolithic ALE computations of shock hydrodynamics using nodal elements", JCP, 315 (2016), 577-608. [2] Jean-Luc Guermond, Bojan Popov, Vladimir Tomov, "Entropy-viscosity method for the single material Euler equations in Lagrangian frame", CMAME, 300 (2016), 402-426. [3] Guglielmo Scovazzi, Brian Carnes, Xianyi Zeng, Simone Rossi, "A simple, stable, and accurate linear tetrahedral finite element for transient, nearly, and fully incompressible solid dynamics: A dynamic variational multiscale approach", IJNME, 106 (10) (2016), 799-839.

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Title: An Interfacial Zone Model for Intercellular Interaction Modeling in Epithelial Cells

Author(s): *Xiaowei Zeng, *Univ of Texas at San Antonio*; Liqiang Lin, *University of Texas at San Antonio*.

Cell migration plays a pivotal role in many physiological processes including morphogenesis, wound healing as well as tumor metastases. During collective cell migration, the cell-cell interaction will significantly affect the collective migratory behaviors. Recent experimental observation indicated that the intercellular adhesion sites within a migrating monolayer are subjected to both normal stress exerted perpendicular to cell-cell junction surface and shear stress exerted tangent to cell-cell junction surface. Based on this observation, we developed an interfacial zone model to model the intercellular interactions in normal and tangential directions at the cell-cell junction surface. Simulation results revealed that the value of average normal stress was greater than that of maximum shear stress, which might be the reason that cell-cell junction carries dominant loading perpendicular to intercellular surface due to “adhesive belt” formed by concentration of E-cadherin. Also, there was a strikingly coincidence with the experimental observation that the orientation of local principal stress was in alignment with that of migration velocity vector, which indicated that cells will migrate along orientations of minimal intercellular shear stress. Our simulation results might help explain the recently discovered “plithotaxis” mechanism in collective cell motion.

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Title: A Double-Layer Interpolation Method for BIE Implementation

Author(s): *Jianming Zhang, Weicheng Lin, Yunqiao Dong, Chuanming Ju, *Hunan University*.

By combining the conventional polynomial element interpolation and the moving least-square (MLS) interpolation, a double-layer interpolation method (DLIM) is proposed for boundary integral equation (BIE) implementation. In the DLIM, the nodes of an element are sorted into two groups: (i) nodes inside the element, which are called source nodes; and (ii) that on the vertices and edges of the element, which are called virtual nodes. With only the source nodes, the element turns to be a conventional discontinuous element. With both the source nodes and the virtual nodes, the element becomes a standard continuous element. The physical variables are interpolated by the continuous element (first layer interpolation) while the BIE is collocated at the source nodes, only. We further build relationship between the source nodes and the virtual nodes using the MLS. With these relations, we finally obtain a square matrix for the overall system of linear algebraic equations. Our method will significantly increase the computational accuracy at equivalent computational cost as those using discontinuous elements. Moreover, by manipulating the influence domains of some specific nodes in the MLS, the DLIM will be able to accurately and naturally interpolate both continuous fields (potential for example) and discontinuous fields (normal flux for example). Because of this feature, our method can be easily extended to solve problems involve discontinuity, such as crack propagation, contact problems, etc. Numerical examples are presented to show the accuracy and convergence rate of our method.

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Title: Layout Optimization of Magnetorheological Fluid Patches in Plate Structures by Using Semi-Active Control

Author(s): *Xiaopeng Zhang, *Dalian Univ. of Tech., China* ; Akihiro Takezawa, *Hiroshima University, Japan*; Zhan Kang, *Dalian University of Technology, China* .

We present the topology optimization of the magnetorheological fluid material layout in a sandwich plate for reducing the structural vibration level under harmonic excitations. Therein, the magnetorheological fluid layer, consisting of a cluster of MR ■uid segments, is placed for providing semi-active damping control effect under a uniform magnetic field. In the topology optimization model, the aggregated dynamic compliance in a given frequency range is taken as the objective function. The pseudo-densities describing the MR ■uid segments distribution are taken as the design variables, and a penalization model on the shear stiffness of the MR fluid is employed. In this context, the adjoint-variable sensitivity analysis scheme is derived. The effectiveness and efficiency of the proposed method are demonstrated by numerical examples, and several key factors on the optimal designs are also discussed.

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Title: Explicit Three Dimensional Topology Optimization via Moving Morphable Component/Void (MMC/MMV) Approach

Author(s): *Weisheng Zhang, *Dalian University of Technolog*; Jishun Chen, Xu Guo, *Dalian University of Technology*.

Three dimensional (3D) topology optimization problems always involve huge numbers of Degrees of Freedom (DOFs) in finite element analysis (FEA) and design variables in numerical optimization. This will inevitably lead to large computational efforts in the solution process. In the present paper, an efficient and explicit topology optimization approach which can reduce not only the number of design variables but also the number of degrees of freedom in FEA is proposed based on the Moving Morphable Component/Void (MMC/MMV) solution framework. In the MMC/MMV approach, the topological change of a structure is achieved by the deformation, intersection and merging of a set of closed parametric curves (for 2D problems) or parametric surfaces (for 3D problems) that represent the boundary of the structure. Unlike the traditional level set approach, there is no need to introduce an extra level set function defined in a higher dimensional space to represent the structural boundary implicitly in the MMC/MMV approach. This greatly reduced the number of design variables involved in the optimization problem. In the present explicit boundary evolution-based approach, the computational effort associated with FEA can be reduced substantially by removing the unnecessary DOFs from the FE model at every step of numerical optimization. Numerical examples demonstrate that the proposed approach does can overcome the bottleneck problems associated with a 3D topology optimization problem in a straightforward way and enhance the solution efficiency significantly.

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Title: Material Properties and Morphology Parameters Sensitivity Analysis in Energetic Material

Author(s): *Xiaoyu Zhang, Caglar Oskay, *Vanderbilt University*.

We present a novel parameter sensitivity analysis framework for damage and failure modeling of particulate composite materials subjected to dynamic loading. The proposed framework is employed to quantify the sensitivity of the failure response of energetic materials (e.g., explosives, propellants) under dynamic loads to both material properties and morphological parameters that define the material microstructure. The proposed framework employs global sensitivity analysis (GSA) to study the decoupling of the uncertainty or variance in the failure response as a function of model parameter uncertainty. In view of the computational complexity of performing thousands of detailed microstructural simulations to characterize sensitivities, a Gaussian Process (GP) surrogate modeling is incorporated into the framework. The GP model is built on Gaussian kernels, and approximates the response surface generated by directly resolution finite element analysis with an extremely low cost mapping function. In order to capture the discontinuity in response surfaces, the GP models are integrated with a classification algorithm that identifies the discontinuities within response surfaces. A support vector machine (SVM) classifier is trained to obtain a separating hyperplane. The proposed framework is employed to quantify variability and sensitivities in the failure response of particular energetic materials with a polymeric binder (PBX). The failure behavior is characterized with thermo-mechanical analyses at the scale of the material microstructure. Particular emphasis is placed on the identification of sensitivity to interfaces between the polymer binder and the energetic particles. The proposed framework has been demonstrated to identify the most consequential materials and morphological parameters under vibrational and impact loads.

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Title: Sparse and Scalable Eigenstrain-Based Reduced Order Homogenization Models for Polycrystal Plasticity

Author(s): *Xiang Zhang, Caglar Oskay, *Vanderbilt University*.

We present an accelerated, sparse and scalable eigenstrain-based reduced order homogenization modeling approach for computationally efficient multiscale analysis of polycrystalline materials. The proposed approach is based on the eigenstrain-based reduced order homogenization model (EHM) for polycrystalline materials [1] that concurrently links the response of the structural scale to the response at the scale of the grains and provides significant efficiency in analysis of structures composed of complex polycrystalline microstructures. EHM operates in a computational homogenization setting, and employs concepts from the transformation field theory to pre-compute certain microscale information (e.g. localization tensors, concentration tensors) by evaluating linear elastic microscale problems prior to a macroscale simulation. By this approach, a significant reduction in computational cost is achieved, compared with classical computational homogenization approaches that employ crystal plasticity finite element (CPFE) simulation to describe the microscale response. While EHM provides approximately two orders of magnitude efficiency compared with CPFE for middle-sized microstructures, its efficiency degrades as microstructure size increases. A grain-cluster accelerated, sparse and scalable reduced order homogenization model has been developed to address this issue. The acceleration is achieved by introducing sparsity into the linearized reduced order system through selectively considering the interactions between grains based on the idea of grain clustering. The proposed approach results in a hierarchy of reduced models that recovers eigenstrain-based homogenization, when full range of interactions are considered, and degrades to the Taylor model, when all inter-grain interactions are neglected. The resulting sparse system is solved efficiently using both direct and iterative sparse solvers, both of which show significant efficiency improvements compared to the full EHM. A layer-by-layer neighbor grain clustering scheme is proposed and implemented to define ranges of grain interactions. Performance of the proposed approach is evaluated by comparing the results against the full EHM and crystal plasticity finite element (CPFE) simulations. [1] X. Zhang and C. Oskay. Eigenstrain based reduced order homogenization for polycrystalline materials. Comput. Methods Appl. Mech. Engrg., 297:408–436, 2015.

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Title: Computational Modeling of the Formation and Mechanical Instability of Solid Electrolyte Interphase on Silicon Electrodes in Lithium-Ion Batteries

Author(s): *Xiaoxuan Zhang, Christian Linder, *Stanford University*.

Lithium-ion batteries (LIBs) are important energy storage devices for portable electronics and are growing in popularity for electric vehicles due to their high energy capacity. Also, the electric vehicle industry persistently requires batteries with higher energy capacity, higher energy capacity and longer cycle life. One of the known methods to improve LIBs' energy capacity is to use new electrode materials. Silicon (Si) is an attractive electrode material with a maximum theoretical specific capacity of 4200mAh/g, compared with 372mAh/g for graphite used in commercial Lithium-ion batteries. However, enormous volume changes (~310% at full lithiation of Si) caused by the insertion and extraction of Lithium (Li) lead to mechanical failure, chemical degradation and capacity loss of Si electrodes. The charging and discharging process of Si electrodes is a complex process involving phase transformation and electro-chemo-mechanical coupling. In our previous research, we developed a reaction-controlled diffusion model [1] to describe the evolution of the phase boundary in Si electrodes and a chemo-mechanical coupled computational framework [2] to investigate the diffusion induced anisotropy and fracture in Si electrodes. Based on this framework, in this work, we will investigate the formation mechanism and mechanical instability of solid electrolyte interphase (SEI) on Si electrodes. The SEI layer is a thin layer formed at the interface between the negative electrode and the electrolyte in LIBs due to the irreversible electrochemical decomposition of the electrolyte material. Its formation consumes active material and electrolyte and is one of the key factors affecting the lifetime and safety of LIBs. Here, we will present a growth model for the SEI layer. We use the phase field model for fracture and the cohesive zone model to study the mechanical instability of the SEI layer. We show how the SEI layer is related to electrode capacity loss. We further show how its mechanical instability is affected by electrode geometries and battery operational conditions. References: [1] X. Zhang, S. Lee, H. Lee, Y. Cui, C. Linder, A reaction-controlled diffusion model for the lithiation of silicon izn lithium-ion batteries. Extreme Mechanics Letters. (2015) 4:61-75. [2] X. Zhang, A. Krischok, C. Linder, A variational framework to model diffusion induced large plastic deformation and phase field fracture during initial two-phase lithiation of silicon electrodes, Computer Methods in Applied Mechanics and Engineering, (2016), 312:51-77.

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Title: Development and Applications of the Discrete Adjoint Solver in PETSc

Author(s): *Hong Zhang, Emil Constantinescu, *Argonne National Laboratory*.

Sensitivity analysis is crucial to identify the most influential parameters in simulations, to describe the behavior of dynamical models, and to solve dynamic constrained optimization problems. Existing easy-to-implement approaches such as finite-difference and forward sensitivity analysis require a computational effort that increases linearly with the number of sensitivity parameters. In this work, we investigate, implement, and test a discrete adjoint approach [1], whose computational effort is effectively independent of the number of sensitivity parameters. The approach is highly efficient for calculating sensitivities of larger systems and is consistent with the function whose sensitivity we are seeking. This is an essential feature for use in optimization applications. Moreover, our approach includes a consistent treatment of dynamical systems with switching by deriving and implementing the adjoint jump conditions that arise from state- and time-dependent switchings. An efficient implementation of our approach has been developed as part of the time-stepping component in PETSc. By design, it takes advantage of the highly scalable lower-level components such as nonlinear/linear solvers, preconditioners and parallel data structures; it can also be used in some higher-level software such as the optimization library TAO and the PDE library libMesh. We will demonstrate the capability of the discrete adjoint solver for complex power grid simulations. Due to the generality of the framework, many other applications, especially existing ones using PETSc, would be expected to benefit from this development with minimum user effort. References [1] Hong Zhang, Shrirang Abhyankar, Emil Constantinescu, Mihai Anitescu. Discrete adjoint sensitivity analysis of hybrid dynamical systems with switching, IEEE transaction on Circuits and Systems I, in press, 2017

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Title: A Multi-Scale Modeling of Strain Path Effects, Laminar Structure and Texture Evolution in Wire Drawing Process

Author(s): *Guangliang Zhang, *taizhou university*.

In steel wire drawing, the material in the wire core and surface experiencing different strain paths due to the effect of die geometries, will present significant difference in the lamella structure, texture and the mechanical properties, which is referred to as the strain path effects. As taking strain path as a breakthrough, this research is aimed at developing an accurate finite element model of multi-pass wire drawing for the strain path analysis; a multi-scale model involving the strain path modeling, the lamella deformation modeling, and the texture modeling; as well as characterizations of the lamellar structure and texture and measurements of the gradient mechanical properties by considering the strain path effects. It aims at studying the mechanisms in the strain path evolution, the effects of strain path on lamella structure deformation, texture evolution and mechanical properties between wire core and surface. Based on the new developed strain path effects theory, it will open a new gate to develop super high strength wires with better control of the strain path and microstructure evolution.

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Title: Modeling of the Periodic Axon Membrane Skeleton Structure with Measurement of Its Mechanical Properties

Author(s): *Yihao Zhang, Krithika Abiraman, David Pierce, Anastasios Tzingounis, George Lykotrafitis, *University of Connecticut*; He Li, *Brown University*.

It has been recently shown by super-resolution microscopy experiments that unlike the soma and dendrites, the axon membrane skeleton comprises a series of actin rings connected by extended spectrin filaments with a periodic distance of 180nm to 190nm. Sodium channels, which are associated with spectrin via ankyrin, also exhibit a periodic distribution pattern. In our work, we first showed, by using atomic force microscopy, that the stiffness of the axon plasma membrane is significantly higher than those of dendrites and somata. Then, we developed a coarse-grain molecular dynamics model of the axon membrane skeleton to investigate its effect on the overall stiffness of the axon. The proposed model accurately represents the stiffness of the axon membrane by comparing the median value of its Young's modulus to the result determined by atomic force microscopy. Also, the model predicts that the spectrin filaments are under entropic tension. We concluded that the thermal random motion of the voltage-gated sodium channels, which are bound to ankyrin particles, is reduced compared to the thermal motion when spectrin filaments are held at equilibrium. Finally, we predicted that the injuries leading to laceration of spectrin filaments can cause a permanent damage to the axon membrane skeleton due to the fact that spectrin filaments are under tension and once they are disrupted they cannot spontaneously re-form their initial configuration. We expect that the model can be used to study the mechanical stability of the axon.

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Title: A Multi-Temporal Scale Approach To Thermomechanical Failure And Response Prediction

Author(s): *Rui Zhang, Dong Qian, *University of Texas at Dallas*; Lihua Wen, Jinyou Xiao, *Northwestern Polytechnical University*.

In this work, we present a computational approach to thermomechanical failure and response prediction with an efficient solver employing time-discontinuous Galerkin (TDG) based space-time finite element method and its enriched version (XTFEM) [1-3] in three dimensions. While the robustness of TDG based space-time FEM has been extensively demonstrated, a critical barrier for the extensive application is the large computational effort due to the additional temporal dimension and enrichment that are introduced. By formulating a new preconditioner and utilizing the properties of Kronecker product, we developed a generic iterative algorithm for solving the fully-coupled block-structured matrix equations formulated by space-time FEM. This approach reduces the computational cost to the same order of solving the corresponding static problems. The established numerical framework is further integrated with a thermomechanical damage model for the purpose of capturing failure initiation and propagation. The efficiency and robustness of the proposed method are illustrated in numerical examples, in which we show much better performance over direct solution of the original TDG matrix equations using either sparse direct or iterative solvers [1] Y. Yang, S. Chirputkar, D. N. Alpert, T. Eason, S. Spottswood, and D. Qian, "Enriched space-time finite element method: a new paradigm for multiscaling from elastodynamics to molecular dynamics," International Journal For Numerical Methods In Engineering, vol. 92, pp. 115-140, Oct 12 2012. [2] S. Bhamare, T. Eason, S. Spottswood, S. R. Mannava, V. K. Vasudevan, and D. Qian, "A multi-temporal scale approach to high cycle fatigue simulation," Computational Mechanics, vol. 53, pp. 387-400, 2014. [3] R. Zhang, L. Wen, S. Naboulsi, T. Eason, V. K. Vasudevan, and D. Qian, "Accelerated multiscale space–time finite element simulation and application to high cycle fatigue life prediction," Computational Mechanics, vol. 58, pp. 329-349, 2016.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Modeling Hydraulic Fracture Height Growth and Proppant Transport in a Formation with Stress Drop

Author(s): *Fengshou Zhang, *Tongji University*; Egor Dontsov, *University of Houston*.

The goal of this presentation is to study hydraulic fracture height growth and proppant transport in a multi-layer formation with stress drop using a 3D distinct element code 3DEC. The numerical scheme takes into account the coupling between the viscous fluid flow and elastic interactions, while the fracture propagation is modeled by a modified tensile strength criterion that accurately captures the fracture toughness and considers the mesh size effect. The presence of proppant in the fracturing fluid is modeled by its volumetric concentration. The effects of proppant “pack”, which corresponds to the situation when the concentration reaches a given threshold value, and “bridging”, when the fracture aperture is sufficiently small to permit further proppant movement, are both included into the model. Proppant pack is able to sustain the load from the closing fracture and only the fracturing fluid is able to penetrate through the pores of the pack. In order to validate the model, 3DEC is used to simulate the radial hydraulic fracture in the viscosity dominated regime, toughness dominated regime and the intermediate regime. The modeling results are compared to the theoretical solutions and showed good agreement. Then, the multi-layer hydraulic fracture height growth is modeled with and without proppant, where the stress drop is introduced above the primary layer. The fracture initially propagates as a radial crack from the injection point. The hydro-mechanical coupling results in pinching and smaller aperture at the interface between the stress layers. The fracture has a tendency to propagate upward rapidly once it reaches the stress drop, which requires a large volume of fluid to fill the rapidly opening fracture. However, the increased pressure gradient in the bottom layer associated with the larger flow speed results in smaller net pressure and causes the pinch. Depending on the proppant size, proppant could be “bridged” along the interface of stress drop, which causes a significant decrease of fluid supply into the upper layer. The results indicate that the effect of proppant could be significant at the interface of stress drop. It is therefore necessary to consider the coupling between the proppant, fluid, and rock for the modeling of fracture height growth.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Topology Optimization of Incompressible Solids under Finite Deformation

Author(s): *Guodong Zhang, Kapil Khandelwal, *University of Notre Dame*.

A framework for topology optimization of incompressible media in the context of finite deformation is proposed. Several challenges pertaining to the problem are discussed and addressed, including: (a) proper measurement of element distortion for ensuring the correctness of solution of finite element analysis (FEA); (b) strategies for dealing with excessive distortion of low-density elements under large deformation; (c) the use of advanced finite elements for handling incompressibility constraints; (d) appropriate material interpolation schemes for incompressible materials under large deformation. In particular, FEA solutions with highly distorted element(s), would lead to incorrect sensitivity information and further lead to unreal update in topology. In addition, the low-density elements might experience excessive distortion under large deformation, which will result in the non-convergence in FEA. Moreover, the appearance of volumetric locking in FEA would cause dramatic changes in the topology optimization, which is also demonstrated through examples. To address these issues topology optimization of incompressible media is addressed in a density-based approach using fictitious domain method [1] in which the method of moving asymptotes (MMA) is adopted as the optimizer. Furthermore, in constructing the material interpolation schemes, the incompressibility of low and intermediate density elements is addressed. Several commonly used hyperelastic materials including Ogden model, Mooney-Rivlin model and Neo-Hookean model are considered. Multiple topology optimization problems are examined to show the effectiveness and robustness of the proposed methods. Finally, the optimized topologies for compressible and incompressible solids are compared. References: [1] Wang, F., Lazarov, B., Sigmund, O., and Jensen, J. (2014) “Interpolation scheme for fictitious domain techniques and topology optimization of finite strain elastic problems”, Computer Methods in Applied Mechanics and Engineering, Vol. 276, Pages 453-472, doi: 10.1016/j.cma.2014.03.021. Keywords: Topology optimization; Finite deformation; Incompressible media; Hyperelastic materials.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Integrating CAD with Abaqus: A Practical Isogeometric Analysis Software Platform for Industrial Applications

Author(s): *Jessica Zhang, *Carnegie Mellon University*.

Isogeometric analysis (IGA) has been developed for more than a decade. However, the usage of IGA is by far limited mostly within academic community. The lack of automatic or semi-automatic software platform of IGA is one of the main bottlenecks that prevent IGA from wide applications in industry. In this talk, we present a comprehensive IGA software platform that allows IGA to be incorporated into existing commercial software such as Abaqus, heading one step further to bridge the gap between design and analysis. The proposed IGA software framework takes advantage of user-defined elements in Abaqus, linking with general .IGES files from commercial computer aided design packages, Rhino specific files and mesh data. The platform includes all the necessary modules of the design-through-analysis pipeline: pre-processing, surface and volumetric T-spline construction, analysis and post-processing. Several practical application problems are studied to demonstrate the capability of the proposed software platform.

14th U.S. National Congress on Computational Mechanics
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Title: Data-Driven Probabilistic Calibration of Material Models from Small Datasets and Its Influence on Structural Response

Author(s): *Jiaxin Zhang, Aakash Bangalore Satish, Michael Shields, *Johns Hopkin University*; Pawel Woelke, *Thornton Tomasetti – Weidlinger Applied Science*.

Abstract Most structural-scale material models are empirical or phenomenological and require calibration from experimental material data. This calibration process is complicated when material properties are variable/uncertain. A principle challenge in this case is that experimental data are typically scarce since mechanical tests are usually time-consuming and often expensive, particularly under extreme conditions such as high temperature and/or high strain rates. This paper proposes a data-driven approach for material model calibration from small datasets. The methodology incorporates the full uncertainty associated with probability model form and parameter estimation for material constitutive parameters. This is achieved by utilizing multimodel inference to identify plausible candidate probability models and Bayesian inference to estimate the model parameters. Incorporating these influences results in an imprecise probabilistic model that provides a more realistic assessment of the uncertainties associated with the material performance and structural response than classical calibration procedures. The proposed calibration methodology is applied for probabilistic parameter estimation for material behavior represented by a temperature dependent viscoplastic damage model for ductile metals [1-2]. Particularly, the model is calibrated for aluminum alloy Al-6061 T6 at temperatures ranging from room temperature to 300C to model structural response during fire. A set of mechanical tests of Al-6061 T6 at various temperatures have been conducted to collect material data that are used for material model calibration. The calibrated material model is implemented in ABAQUS as a VUMAT and simulations of aluminum structural components during fire conditions are performed. We assess uncertainties in the structural response with an aim at placing realistic bounds on their reliability. Probabilistic structural modeling is conducted using an efficient Bayesian importance sampling method for propagating the imprecise probabilities associated with material parameters [3]. References [1]. P.B. Woelke and N.N. Abboud, 2012. Modeling fracture in large scale shell structures. Journal of the Mechanics and Physics of Solids, 60(12), pp.2044-2063. [2]. P.B. Woelke, M.D. Shields, N.N. Abboud and J.W. Hutchinson. 2013. Simulations of ductile fracture in an idealized ship grounding scenario using phenomenological damage and cohesive zone models. Computational Materials Science, 80, pp.79-95. [3]. J. Zhang and M.D. Shields. 2017. On the quantification and efficient propagation of imprecise probabilities resulting from small datasets. Mechanical Systems and Signal Processing (In Review).

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: The Effect of Residual Stress on Stress-Modulated Growth in an Artery

Author(s): Jie Cheng, *Rensselaer Polytechnic Inst.*; *Lucy Zhang, *Rensselaer Polytechnic Institute*.

Growth plays a key role in many biological and medical processes, and often takes place under the stimuli of mechanics. Residual stress is known to exist in vessels when it is not under any mechanical loading. As a result, a stress-modulated growth is expected to be largely dependent on the initial stress state or the residual stress. In this talk we examine the impact of residual stress on the growth of arterial wall using a finite element simulation, where the stress-modulated growth is implemented based on the multiplicative decomposition approach. The artery wall is modeled as a multi-layered, anisotropic, hyperelastic tube. Open-angle and axial pre-stretch are applied to generate the residual stress in the artery wall. It is found in this study that different amount of residual stress can affect the stress distribution under a pressure load, thereby change the growth rate of the artery wall. The results indicate that the arterial stenosis might originate from an abnormal distribution of the residual stress. Future studies on multiscale simulations on the generation of the residual stress modulation will be discussed.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Simulations of Gas-Liquid-Solid Interactions Using the Immersed Approach

Author(s): *Lucy Zhang, *Rensselaer Polytechnic Inst.*.

In this talk, we use the immersed approach to model and simulate gas-liquid-solid three-phase flows. The overall algorithm adopts a non-boundary-fitted approach that avoids frequent mesh-updating procedures by defining independent meshes and explicit interfacial points to represent each phase. In this framework, we couple our existing solvers, the immersed finite element method (IFEM) and the connectivity-free front tracking (CFFT) method that model fluid-solid and gas-liquid interactions, respectively, for the three-phase models. A modified IFEM algorithm is used for modeling fluid-solid interactions that accounts for the dynamics of the solid, while the CFFT is used to simulate gas-liquid multiphase flows that uses explicit interfacial points to represent the gas-liquid interface and for its easy handling of interface topology changes. Instead of defining different levels simultaneously as used in level sets, an indicator function naturally couples the two methods together to represent and track each of the three phases. Several 2-D and 3-D testing cases are performed to demonstrate the robustness and capability of the coupled numerical framework in dealing with complex three-phase problems, in particular free surfaces interacting with deformable solids. The solution technique offers accuracy and stability, which provides a means to simulate various engineering applications that involve high Reynolds number flows, large deformations, and high density disparities among the phases.

14th U.S. National Congress on Computational Mechanics
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Title: Combining Continuum Damage With A Cohesive Zone Model: Modeling Damage In Quasi-Brittle Materials With Application To Masonry Structures

Author(s): *Shenghan Zhang, Nicolas Richart, Katrin Beyer, *Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland*.

Quasi-brittle materials (e.g., concrete) normally exhibit two types of failure: (i) diffuse damage and (ii) localized damage. A cohesive zone modelling approach is well suited for simulating localized damage where one or several cracks dominate the failure mechanism. This can be implemented by means of cohesive elements or a mesh-less method. For simulating diffuse damage, a phenomenological continuum damage model is typically employed [1]. Recently, mainly for tensile damage, a unified framework for transformation of diffused damage to localized cohesive zone model has also been proposed [2]. It has been observed that, for quasi-brittle material, different types of failure relate to different loading conditions: the diffuse damage is often observed for compression loading while the localized damage is typically obtained under tension or tension-compression. Based on this observation, we combine cohesive zone model with a continuum damage model to represent the material behavior. This allows to achieve a more realistic representation of damage for different loading conditions. Additionally, for masonry structures, both interfacial debonding (between units and mortar) and damage in the mortar are crucial to the failure mechanism [3]. While interfacial debonding is well represented by cohesive elements, the proposed method also provides a unified way of representing damage both in the interface and in the mortar. In order to consider friction within cohesive elements, a new contact algorithm is further put forward. We present applications of this modelling approach by analyzing unreinforced masonry structures under different loading conditions. References: [1] J. Lee and G. L. Fenves, “Plastic-Damage Model for Cyclic Loading of Concrete Structures,” J. Eng. Mech., vol. 124, no. 8, 1998. [2] Y. Wang and H. Waisman, “From diffuse damage to sharp cohesive cracks: A coupled XFEM framework for failure analysis of quasi-brittle materials,” Comput. Methods Appl. Mech. Eng., vol. 299, pp. 57–89, Feb. 2016. [3] S. Zhang, S. M. Taheri Mousavi, N. Richart, J.-F. Molinari, and K. Beyer, “Micro-mechanical finite element modeling of diagonal compression test for historical stone masonry structure,” Int. J. Solids Struct.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Simulating the Effect of Permanent Set on Bioprosthetic Heart Valves under Cyclic Loading

Author(s): *Will Zhang, Michael Sacks, *University of Texas at Austin*.

There are over 100,000 heart valve surgeries done each year in the U.S. costing over $20 billion. Bioprosthetic heart valves (BHV) are the most popular surgical replacements, but the life expectancy remains stuck at 10-15 years. One of the most crucial effects involved in the mechanical failure of BHVs is permanent set (PS); especially in the early stage (2-3 years). PS cause the geometry of BHVs to change permanently over time, resulting in extraneous stress on the leaflets. While this process does not damage the tissue, it accelerates the rate of failure. PS is a result of the scission-healing of exogenously crosslinked matrix. This allows the unloaded configuration of the matrix to evolve while convecting the underlying collagen fiber architecture (CFA). Thus, we developed a constitutive model for BHVs based on the PS mechanism. The results show that PS alone can capture and more importantly predict how the shape and mechanical response leaflet biomaterial change during the early stage. In this work, we developed a computational implementation to simulate intact BHVs under cyclic loading. We started with the approach of Aggarwal and Sacks [1] and implemented the constitutive model in Finite Elements. Next, we extended the computational model for the time evolving properties due to PS, quasistatically. At each time step, we first simulated the root mean squared deformation at each integration point for 1 heart cycle. The PS of the matrix is then updated based on the deformation at each point and a single rate constant for PS. This is then used to convect the experimentally obtained CFA, which is directly mapped to the mesh [1]. The updated material parameters were then used to compute the deformation for the next time step. The evolving mechanical response is an integration over the strain history at all the time steps. We thus simulated the evolving unloaded geometry of a BHV in response to PS and explored how the leaflet stresses change with respect to the original BHV geometry and material properties. The results shown the importance of accounting for the PS effect on the performance and durability BHVs. References: [1] A. Aggarwal and M.S. Sacks. An inverse modeling approach for semilunar heart valve leaflet mechanics: exploitation of tissue structure. Biomechanics and Modeling in Mechanobiology, 15:909-932, 2016.

14th U.S. National Congress on Computational Mechanics
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Title: Molten Pool Behavior and Solidification Microstructure of Co-Cr-Mo Alloy in Powder-Bed Electron Beam Additive Manufacturing

Author(s): *Yufan Zhao, Yuichiro Koizumi, Kenta Aoyagi, Kenta Yamanaka, Daixiu Wei, Akihiko Chiba, *Tohoku University*.

Electron beam melting (EBM) is a relatively new powder-bed-fusion additive manufacturing (AM), showing the prospect for fabricating the Co-Cr-Mo (CCM) alloy with customized geometries which are widely used in medical field. In particular for medical implants, fine equiaxed grain is desirable for superior fatigue properties. Therefore, it is essential for us to modify material microstructures through regulating EBM parameters to achieve predictable property finally. The direct correlations between EBM parameters and solidification microstructure or forming quality by experimental methods, consumes tremendous time and cost. The understanding of EBM process at mechanism level can make a bridge between them. But the physical phenomena involving in process are not fully understood and inaccurately predictable owing to its highly transient and localized features. Therefore numerical simulation can be a convenient tool to understand the physical phenomena and develop new process strategies without intensive and expensive trial-and-error. In this work, a three-dimensional (3D) numerical model is developed to investigate the molten pool behavior and to predict the microstructure characteristics in the EBM-built CCM alloy. Molten metal is assumed to be Newtonian and incompressible. A three-dimension model of heat transfer and fluid flow during powder-bed-fusion of CCM alloy is developed based on Computational thermo-fluid dynamics (CtFD) simulation, which is based on a finite volume/finite difference approach, can track the front of the molten metal by a volume-of-fluid (VOF) method and predict temperature field, fluid flow and associated molten pool dynamic and solidified bead geometry. With regard to the generation of powder layer, Discrete Element Method (DEM), which enables description of powder bed packing structure, was used to create initial geometry setting for melting process and then the effect of powder layer on fluid flow and thermal field can be investigated. The simulation reveals that Marangoni effect of molten metal primarily determine the fluid flow pattern and the existence of powder layer influences the fluid flow and solidification conditions. The results indicates that the processing parameters have a profound influence on the molten pool shape and in turn the resulted crystal grain structure in the solidified bead. This work shows great prospects of controlling powder-bed fusion process and optimizing microstructure by quantitative simulation, which are important issues in developing EBM-built alloys.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Application of a Time Discontinuous Material Point Method to Transient Problems

Author(s): *Yonggang Zheng, Mengkai Lu, Jiayong Zhang, Hongwu Zhang, *Dalian University of Technolog*; Zhen Chen, *University of Missouri*.

Transient responses of structures to blast or impact loading conditions usually exhibit discontinuity or sharp gradient characteristics and the structures suffer from the severe deformation near the impact or loading area, which may eventually lead to structural failure. Although the material point method (MPM) [1,2] has been widely used to solve these problems, the transient problems involving discontinuity or sharp gradient characteristics have still not been well handled with the existing MPM-based methods. In our present work, based on the strength of the time-discontinuous Galerkin formulation [3], we propose a time-discontinuous material point method (TDMPM) to better simulate these transient problems. In the TDMPM, the continuous time domain is divided into discrete time intervals. By considering the discrete grid governing equations, the constraint and discontinuity conditions, the weak form of the TDMPM is derived. The displacement and velocity fields in each time interval are interpolated by the corresponding values at the two time instants that enclose the time interval via the piecewise cubic and linear functions, respectively. By substituting the assumed displacement and velocity fields into the weak form, a novel computational framework for updating the grid displacements and velocities at discrete time instants is set up. In the new formulations, the displacement field at each time instant remains to be continuous, whereas the velocity field at the corresponding time instant becomes discontinuous. These features ensure that the TDMPM can properly capture the discontinuous characteristics and suppress the spurious numerical oscillations. Several representative examples demonstrate that the proposed TDMPM is efficient and accurate. Moreover, this method could be easily implemented into the programs for the original MPM. This work was supported by the National Natural Science Foundation of China (11672062 and 11232003) and the Fundamental Research Funds for the Central Universities (DUT14YQ217). [1] D. Sulsky, Z. Chen, H.L. Schreyer, A particle method for history-dependent materials, Comput. Methods Appl. Mech. Engrg. 118 (1994) 179–196. [2] Y.G. Zheng, F. Gao, H.W. Zhang, M.K. Lu, Improved convected particle domain interpolation method for coupled dynamic analysis of fully saturated porous media involving large deformation, Comput. Methods Appl. Mech. Engrg. 257 (2013) 150–163. [3] X.K. Li, D.M. Yao, R.W. Lewis, A discontinuous Galerkin finite element method for dynamic and wave propagation problems in non-linear solids and saturated porous media, Int. J. Numer. Methods Engrg. 57 (2003) 1775–1800.

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14th U.S. National Congress on Computational Mechanics
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Title: Rotation-Free Triangle and Its Application in Dynamic Drape Simulation

Author(s): *Yexin Zhou, *1. Tongji Univ 2. Jiangsu Univ*; Kam yim Sze, *The University of Hong Kong*.

Drape simulation finds its applications in fashion design, e-commerce of clothing and production of animated movies. Fabric drapes are typical large displacement, large rotation and small strain problems. Compared with the conventional geometric non-linear shell analysis, computational drape analysis is particularly challenging due to the small bending to tensile rigidity ratio of most fabric. The task has been undertaken by different approaches which include but not restrict to particle methods, finite element methods and rotation-free element methods. In this presentation, a rotation-free triangle will be presented. Its bending response is based on a six-node quadratic interpolation of displacement using an overlapping element concept and is extended to large displacement/rotation analyses by using a corotational framework. The triangle is particular efficient in the sense the tangential bending stiffness matrix is a constant which does not need to be updated. On the other hand, its membrane energy is considered by the CST approximation. Despite of its simplicity and efficiency, its accuracy is competitive with respect to other rotation-free triangles in the literature [1]. While the triangle works fine in static drape problems, non-physical folds are sometimes predicted if the product of the curvature and the element size is excessive. The cause is traced to be a zero energy mode caused by the CST approximation. The drawback is rectified by also using the six-node displacement interpolation in deriving the membrane strain [2]. An adaptive remeshing scheme is developed for efficient prediction of deep folds. The triangle has been successfully applied to simulations of dynamic drape, dynamic contact, fabric over a walking manikin, etc [2,3]. References Zhou YZ, Sze KY (2012). A geometric nonlinear rotation-free triangle and its application to drape simulation. Inter.J. Numer.Methods Engrg. 89: 509-536. Sze KY, Zhou YX (2016) An efficient rotation-free triangle for drape/cloth simulations - Part I: model improvement, dynamic simulation and adaptive remeshing. Inter.J.Comput.Methods, 13(3): 1650021 (27 pages). Sze KY, Zhou YX (in preparation) An efficient rotation-free triangle for drape/cloth simulations - Part II: collision handling and garments on manikins.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Formulation of Governing Equations in Piezoelectric and Piezomagnetic Materials Directly Using the Law of Conservation of Energy

Author(s): *Peng Zhou, *Harbin Institute of Technology*.

Governing equations in piezoelectric and piezomagnetic materials are usually formulated using the Lagrangian approach. Two extra energy terms, which are proportional to the elastic strains, the electric and magnetic fields, are assumed to be associated with these two processes. However, there is a sign change of these energy terms when either strains or the electric and magnetic fields switch directions. In this paper, a new approach which directly uses the law of conservation of energy (LCE) is proposed. First, for the uncoupled elastic and electromagnetic (EM) processes, it is shown both governing equations satisfy the LCE, respectively. Then, for the coupled piezoelectric and piezomagnetic processes, when substituting the constitutive equations for the direct effects into the LCE for the EM fields, extra terms which representing the conversion of energies are identified. Substitution of these extra terms into the LCE for the elastic fields leads to the constitutive equations for the converse effects directly. That is, the constitutive equations for both the direct and converse effects guarantee the LCE is satisfied. Most importantly, using this new approach, the piezoelectric and piezomagnetic processes are found to be associated with two extra work terms rather than energy terms. The rates of these work terms are proportional to the rate of change of elastic strains. Physical explanations are further provided to help understanding the processes of conversion of energies via these work terms. With this new approach, the energies converted can be numerically evaluated to facilitate the design of piezoelectric and piezomagnetic devices.

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Title: A 3D Immersed Boundary Method for Viscoelastic-Fluid-Structure Interaction

Author(s): *Luoding Zhu, *Indiana University - Purdue Un*.

Fluid-structure-interaction (FSI) is complex and challenging to model and simulate, and it is still an area of active research. Motivated by FSI phenomena in life sciences (e.g., motions of sperm and cytoskeleton in complex fluids), we introduce a new immersed boundary method for FSI problems involving viscoelastic fluids in three dimensions. The viscoelastic fluids are modelled by the FENE-P model (including the Oldroyd-B model as an especial case) and numerically solved by a lattice Boltzmann scheme [1] (the D3Q7 model). The fluid flow is modelled by the lattice Boltzmann equations and numerically solved by the D3Q19 model [2]. The deformable structure and the fluid-structure-interaction are handled by the immersed boundary method [3]. As an application, we consider a simple FSI toy problem - interaction of an elastic flag (fixed at its leading edge and restricted nowhere else) with a viscoelastic fluid in a 3D flow tunnel. No-slip boundary condition is applied on the top, bottom, front, and rear walls. Velocity is given as a constant on the inlet plane and no-friction condition is applied on the outlet plane. Drag of the flag is computed, drag scaling is studied, and effects of several dimensionless parameters on drag and its scaling are investigated. References: 1. Malaspinas, O., N. Fietier, and M. Deville, Lattice Boltzmann method for the simulation of viscoelastic fluid flows. Journal of Non-Newtonian Fluid Mechanics, 2010. 165(23): p. 1637-1653. 2. Zhu, L., et al., An immersed boundary method based on the lattice Boltzmann approach in three dimensions, with application. Computers & Mathematics with Applications, 2011. 61(12): p. 3506-3518. 3. Peskin, C.S., The immersed boundary method. Acta Numerica, 2002. 11: p. 479-517.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: B++ Spline-Based Extended Isogeometric Analysis for Strong and Weak Discontinuities

Author(s): *Xuefeng Zhu, Kai Jiang, Ping Hu, *Dalian University of Technolog*.

We proposed a B++ spline-based eXtended Isogeometric Analysis (XIGA) method to solve the problems with strong or weak discontinuities. The presented method is capable of an efficient analysis of general crack problems and weak discontinuous problems using B++ spline basis as basis functions for both the solution field approximation and the geometric description, and it can reproduce crack tip singular fields and discontinuity across a crack. For crack problems with strong discontinuities, the enriched functions have explicit physical meanings. Also, the proposed method does not require using Lagrange multiplier method, which is often used to impose essential boundary conditions in XIGA or XFEM. Because B++ spline basis functions satisfy the Kronecker delta property, we can strongly impose essential boundary conditions. B++ splines can integrate the boundary curves/surfaces and the background meshes into a unify representation. Hence, for the problem with weak discontinuities, we don't require constructing the implicit function, which is often used to represent the interface. Several numerical examples about crack and multi-materials are presented to verify the efficiency of our method.

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Title: Principal Interval Decomposition Framework for POD Reduced-Order Modeling of Shallow Water Flows

Author(s): *Jean-Marie Zokagoa, *École de Technologie Supérieur*; Azzeddine Soulaïmani, *École de Technologie Supérieure*.

The proper orthogonal decomposition (POD) method is one of the most widely used methods for science and engineering applications to reduce large systems of nonlinear ODEs or PDEs. Good approximations can be obtained with very few POD modes for smooth flow systems. But, when dealing with convective systems, propagation phenomena, and highly nonlinear and unsteady problems, POD models tend to lose their effectiveness because of their use of a time-constant basis. The principal interval decomposition (PID) method can be considered as a strategy to construct more representative basis functions. The key idea in the PID procedure is the use of time subintervals to allow the basis to change with time so that the obtained spatial modes more closely represent a given phenomenon. In fact, using shorter time windows to build the PID-POD basis thus allows the capture of small spatial scales that are missed in standard POD approximations. In the present work, we study the impact of choosing the time subintervals over which POD bases are calculated on the POD-ROM's accuracy in the reduction of shallow water equations (SWEs). The numerical applications are concerned with flood flows on a flat bathymetry, or with a singular bump and flood flows on a natural river bathymetry. The PID/ROM technique significantly improves the predictions compared to the standard POD/ROM. Appreciable speedup (at least 78 times faster) in the calculations is also achieved, compared to the full-order direct numerical simulation using a finite volume model. Errors in the predictions of the water depth found via the standard POD/ROM are reduced by about using the PID procedure. A sensitivity analysis conducted by simultaneously varying the inflow flux and the Manning roughness coefficient on a real bathymetry gives satisfying results. This numerical assessment of the PID technique shows so that it is possible to envisage the use of the PID-POD/ROM technique to build a surrogate model for Monte Carlo-type uncertainty analysis. References Zokagoa, J.-M. and Soulaïmani A. 2011. A POD-based reduced-order model for free surface shallow water flows over real bathymetries for Monte-Carlo-type applications. CMAME, 221-222: 1-23. Zokagoa, J.-M. and Soulaïmani A. 2012. Low-order modelling of shallow water equations for sensitivity analysis using proper orthogonal decomposition. INT J COMPUT FLUID D, 26 (5): 275-295. IJzerman, W. L. (2000). Signal representation and modeling of spatial structures in fluids, Universiteit Twente.

14th U.S. National Congress on Computational Mechanics
July 17-20, 2017, Montreal, Quebec, Canada

Title: Applying Isogeometric Blended Shells to U-Spline Surfaces

Author(s): *Zhihui Zou, Michael Scott, *Brigham Young University*; Derek Thomas, *Coreform LLC*; Bastian Oesterle, Manfred Bischoff, *University of Stuttgart*; Tom Hughes, *The University of Texas at Austin*.

In this talk we will describe our efforts to extend the isogeometric blended shell framework to a newly developed spline representation called U-splines. In our isogeometric blended shell formulation, we avoid a direct interpolation of the increment of the director and instead only approximate the derivatives of the displacement. This leads to improved accuracy in the presence of curved geometry. We also explore the addition of recently proposed hierarchic Reissner-Mindlin shell formulations to the blended shell description. This allows for the elimination of shear locking in both the thick and thin shell regimes and results in improved shear stress representation. We will also describe the application of isogeometric shells to U-spline surfaces. A U-spline overcomes the analysis-suitability restrictions of a T-spline while preserving the mathematical properties required by analysis. We demonstrate the effectiveness of the approach on several carefully selected numerical benchmarks. Keywords: shells, isogeometric analysis, Reissner-Mindlin, Kirchhoff-Love, U-spline

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Title: A Necessary High-Order Meshing Constraint When Using the Finite Element Method on Domains with Curved Boundaries

Author(s): *Philip Zwanenburg, Siva Nadarajah, *McGill University*.

The presented contributions are related to the use of high-order finite element methods using polynomial basis functions for curved geometry representation: 1) Demonstration of the necessity of a high-order meshing constraint (main contribution); 2) Unification of polynomial blending functions for simplex elements; 3) Numerical verification of results for a Poisson problem (Currently working on extending the demonstration to an Euler case). The relation of these results to robustness arises from the harmful impact of improper treatment of curved geometry on high-order simulations. It is well established that the optimal convergence of solutions computed using finite element methods depends on the sufficiently accurate representation of curved boundary geometry when present. The most commonly employed practice for the geometry treatment relies on polynomial approximation of the parameterized boundary surface with subsequent propagation to the interior geometry nodes using blending-function interpolation. Through a geometric proof demonstrating the retention of optimal solution convergence when using 2D polynomial geometry representation, we establish a discrete curvature meshing constraint. Briefly, it is demonstrated that the edge length of elements adjacent to curved domain boundaries must be less than the radius of curvature of the exact boundary before optimal convergence can be observed. We provide numerical verification through a solution to a problem based on the Poisson equation and anticipate obtaining analogous results when solving the Euler equations (currently under investigation), demonstrating the relevance of this meshing criterion in the context of computational fluid dynamics. With the goal of applicability to the most general setting, we also provide numerical results establishing that the optimal convergence is retained on meshes with non-conforming, internally curved edges. While the main result relates to the meshing constraint, several additional contributions arising directly from the proof will also be highlighted. Namely, we demonstrate necessary conditions on 2D surface parameterization and the unification of several successful blending functions for triangular elements within a single framework, potentially providing a simpler alternative to the currently accepted tetrahedral element blending function. While the presentation is only made for the 2D case, the geometric nature of the argument and the generalized form of the blending functions lead to the speculation that an analogous presentation is possible in the 3D setting.