

Using Computational Modeling to Understand Radiation Damage Tolerance in Complex Oxides Both from the Bottom-up and the Top-down

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ABSTRACT

Meeting the ever-increasing demand for energy is a key challenge for the 21st century. Nuclear energy is a proven and green energy source that will be a key component of the world's energy profile. However, maximizing the efficiency of nuclear energy systems, both fission and fusion, requires materials that have significantly increased tolerance against radiation damage. Computational modeling has an important role in understanding and discovering new materials for next-generation nuclear energy systems. In this talk, we will describe research efforts that apply computational modeling to understand the response of materials to radiation damage. We will focus on a class of complex oxides, pyrochlores, that have been proposed for nuclear waste encapsulation. Pyrochlores, with the chemical formula $A_2B_2O_7$, are related to the simpler fluorite structure, with the added complication of having two cation species and oxygen structural vacancies. Past work by numerous groups has shown that the radiation tolerance of these materials is sensitive to the nature of the A and B cations and, in particular, their propensity to disorder. However, these observations are empirical at best and there is still a lack of understanding on the factors that govern the radiation response of these materials. We have tackled this problem from two different perspectives. First, using accelerated molecular dynamics, we have studied how cation disorder, often created during radiation damage, impacts defect kinetics and thus the transport mechanisms that dictate damage recovery. This bottom-up approach has revealed that a percolation transition occurs as disorder is introduced that leads to higher defect mobilities, which in turn promote self-healing of the damage. On the other hand, we have used materials informatics to analyze the role of pyrochlore chemistry on radiation tolerance. In this case, divorced from the complexities of making true predictions of performance, we instead use machine learning to take a top-down perspective and discover heuristic relationships between the material composition and the susceptibility of the material to amorphization. While neither study provides a complete understanding of radiation damage in these materials, together they provide a more complete picture of the factors that dictate their response to irradiation.

Coupled Simulation of Transportation and Electric Power Systems via EVs' Charging Behavior

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ABSTRACT

Realization of a sustainable low-carbon society is required globally, and energy consumption reduction derived from fossil fuels has been emphasized. In the transportation sector, which accounts for a large percentage of energy consumption, EVs (Electric Vehicles) with high environmental performance has been popularized in recent years. To realize a low-carbon society, EVs are expected to play major roles, and it is important to use renewable energy for its charging effectively. Interactions between the road transport network in which gasoline-powered vehicles are used and the electric power system which is maintained by controllable energy systems have not been considered so far. However, the interactions are supposed to occur via EVs, which will popularize in the near future. Most of the previous studies about EVs' popularization focused on either the road transport network or the electric power system, and no sufficient simulation model has been studied for the interaction between both mechanisms. In this research, we proposed a coupled simulation model that can represent interactions between transport and electric power systems. We adopted MATES [1] (Multi-Agent Traffic and Environment Simulator) for simulating the transport mechanism, and implemented an EV agent and its charging behavior. Since the charging event is coupled to the electric power system mechanism, the spread of EVs will affect not only the road transport network but also the electric power system. For simulating the electric power system mechanism, we implemented the BFS (Backward Forward Sweep) method, which is one of the power flow calculation methods for low voltage distribution systems. Numerical experiments are executed in a certain area in the real world. Assuming high-output charging by quick charger at a charging station during long-distance trip and low-output charging by normal charger at home, we evaluated the time series change of the load flow in the urban power system by the EVs' charging events. As a result of the simulation, it was implied that the concentration of low-output charge after returning home might cause a voltage drop in the distribution system. This phenomenon became more prominent as the penetration rate of EV increased, and the possibility that it deviates from the legal range of the reference voltage is shown in some scenarios. [1] S.Yoshimura, "MATES : Multi-Agent based Traffic and Environmental Simulator – Theory, Implementation and Practical Application ", Computer Modeling in Engineering and Sciences, Vol.11, No.1, pp.17-25, (2006)

Development of a Three-dimensional Finite Element Model for a Unidirectional Carbon Fiber Reinforced Plastic Based on X-ray Computed Tomography Images and the Numerical Simulation on Kink Band Failure

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ABSTRACT

A unidirectional carbon fiber reinforced plastic was scanned by an X-ray computed tomography system. Based on the X-ray computed tomography images, a three-dimensional model with random fiber waviness was developed. The constructed three-dimensional fiber model showed random waviness of each fiber in the unidirectional carbon fiber reinforced plastic. Finite element analysis was performed using the three-dimensional model. Simulation results showed bending and twisting deformations coupled with axial contractions during axial compression, which was developed due to fiber waviness. A reduction of the fiber directional Young's modulus due to fiber random waviness was quantitatively evaluated. Propagation of fiber kinking was also studied using the three-dimensional model. Initiation point of the kink-band failure was identified.

Multiscale Study on Origin of Magnetoelectric Effect in Multiferroic Composite Materials

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ABSTRACT

A multiscale numerical investigation into the origin of the magnetoelectric effect in multiferroic composite materials was performed. Specifically, a well-known but unconfirmed mechanism for generating a macroscopic magnetoelectric effect through transmission of mechanical strain between the ferroelectric (FE) and ferromagnetic (FM) phases in an inhomogeneous microstructure was quantitatively established through multiscale finite element simulations. An asymptotic homogenization theory was employed for scale bridging between the macrostructure and the microstructure. Focusing first on a polycrystalline FE/FM composite, the relation between the physical properties and the FE phase content was investigated. Barium titanate was used for the FE phase and Terfenol-D is utilized for the FM phase. The orientation and allocation of FE and FM phases are set to be random. A uniform magnetic field was then applied to the macrostructure and the mechanical strain in the microstructure was investigated. The specific strain component exhibited an off-centered distribution when divided into FE and FM phases. The computation indicated that not only the shift in the mean strain in the microstructure, but also the homogenized piezoelectric stress constant must be increased to enhance the macro magnetoelectric effect. This conclusion is applicable to other inhomogeneous structures and it can explain the trend in the magnitude of the magnetoelectric effect for a random polycrystalline structure, a layered polycrystalline structure, and a layered single-crystal structure. The findings are helpful for the functional design of multiferroic composite materials. One of the authors (Y. Uetsuji) was financially supported by a Grant-in-Aid for Scientific Research (B) (Grant Number 17H03151) from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

Continuum Model of Slow-fast Mode Transition of Crack Propagation in Viscoelastic Materials

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ABSTRACT

The slow-fast mode transition in crack propagation in viscoelastic materials is simulated within the framework of the finite element method (FEM). We successfully reproduced the phenomenon that a discontinuous jump of crack propagation velocity occurs as tensile strain energy increases in rubber and resin. A series of pure shear tests were carried out numerically with FEM simulations and crack velocities were measured under various values of tensile strain. By analyzing the principal stress in the vicinity of the crack tip, it was found that the mode transition is caused by a characteristic temporal change in stress on the crack tip; i.e., non-monotonic increase of stress.

A Molecular Modelling Approach for the Cross-Linking of Nanoparticle-Reinforced Epoxy Resins and Its Effect on Predicted Mechanical Properties

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ABSTRACT

Nanoparticle-reinforced polymers are a novel class of materials and have gained large interest because of their outstanding material properties with respect to stiffness, strength and fracture toughness. Molecular dynamic simulations are an appropriate tool for computational material development and to study the underlying acting mechanisms, since they allow insights into particle-matrix interactions at the atomistic scale [1]. Recent research into the curing process of epoxy resins lead to a simulative cross-linking procedure [2], incorporated into the Molecular Dynamic Finite Element Method (MDFEM) [3] framework and calibrated by experimental in-situ near-infrared spectroscopy data. The calibrated procedure proved to generate simulation models with very good agreement in the curing kinetics and the final network structure. The present work extends the model generation to nanoparticle-reinforced epoxy resins, considering material combinations based on an epoxy system reinforced with boehmite nanoparticles with different partly reactive surface coatings. The present work focuses on two aspects. Firstly, the model generation is investigated, particularly the chemical linkage of the nanoparticle and the epoxy matrix with respect to the surface modifications, in view of the possible chemical reactions between particle and matrix. Since no reaction kinetic is predefined, steric effects and physical interactions, phenomena that are also dominant in reality, govern the bonding. An analysis of the cross-linking process is presented and the effect of the surface modifications on the resultant network structure is investigated. Secondly, material properties of the epoxy-boehmite composite with respect to the particle surface modifications and the particle-matrix interface are evaluated. Effective mechanical properties of the cross-linked nanocomposite are calculated and the correlation to the particle-matrix interaction is discussed. The objective of the contribution is to give an insight into the challenges and opportunities with respect to model generation for molecular dynamics simulations of nanocomposites with the purpose of virtual material development. References [1] Z. Wang et al., Effect of Interfacial Bonding on Interphase Properties in SiO₂/Epoxy Nanocomposite: A Molecular Dynamics Simulation Study, ACS Appl. Mater. Interfaces, 8(11), 2016 [2] R. Unger, B. Daum, U. Braun, R. Rolfes, Experimentally calibrated modelling technique for the cross linking mechanism of epoxy resin and its influence on mechanical properties, Proceedings ICCS20 - 20th International Conference on Composite Structures, 2017, ISBN 9788893850414 [3] L. Nasdala, A. Kempe, R. Rolfes, The molecular dynamic finite element method (MDFEM), CMC: Computers, Materials &&& Continua, 19(1), 2010

Creation of Analysis-Suitable Non-Uniform Rational B-Spline (NURBS) Volumes from Discrete Image-Based Models

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ABSTRACT

In image-based biomedical research, a computer model is obtained by segmenting anatomical structures from medical image data. This typically results in a discrete boundary representation of an anatomy [1]. However, an analytic representation can significantly facilitate engineering design, analysis and computation. Moreover, if the parameterization is analysis suitable, it can enable direct simulation using isogeometric analysis (IGA). Robustly converting a discrete model into an analysis suitable representation is highly challenging and an active area of research [2]. We present a robust and automated method to convert discrete image-based models, particularly for cardiovascular applications, into analysis suitable CAD representations, and demonstrate resulting IGA analysis. Our framework to convert an image-based triangulated surface to a non-uniform rational b-spline (NURBS) volume can be summarized by the following steps: (1) Centerlines of the discrete input model are generated based on an automated cell thinning method creating a graph topology of the model (2) A polycube structure that mirrors this graph topology is generated, providing domains on which NURBS parameterizations will be formed. (3) The input model surfaces are partitioned into patches using the centerlines and centroidal voronoi clustering techniques. (4) Each model patch is mapped conformally to each polycube patch, while ensuring global consistency. (5) Structured parameterizations on the polycube are then mapped back to the original discrete model to provide a structured quadrilateral surface mesh. (6) Interpolation of this surface mesh is used to generate a structured hexahedral mesh volume, which acts as a scaffold onto which an analytic (volumetric NURBS) representation can be formed. The automatic conversion procedure has been tested on a variety of patient-specific vascular models from vascularmodel.org. Final volumetric conversions have been verified with quality metrics such as Hausdorff distance. With a volumetric analytic representation, IGA can be performed, and we will present examples of IGA simulation of blood flow and compare with finite-element modeling. Although these methods were developed primarily for vascular models, they can be utilized on non-vascular geometries that have an identifiable centerline structure as we will demonstrate. Future work includes extending these methods to even more complex anatomies (e.g. beyond genus 0 manifolds). References [1] Updegrove, Adam, et al. "Simvascular: An open source pipeline for cardiovascular simulation." *Annals of biomedical engineering* 45.3 (2017): 525-541. [2] Zhang, Yongjie Jessica. *Geometric modeling and mesh generation from scanned images*. Vol. 6. CRC Press, 2016.

Icing Simulation of NACA0012 Airfoil with Local Surface Heating

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ABSTRACT

Ice accretion is a phenomenon in which super-cooled water droplets impinge and accrete on solid surfaces. In airplanes, this phenomenon reduces the aerodynamics performance or can cause serious accidents. Therefore, de-/anti-icing systems for airfoils have been developed and used up to now, e.g., de-icer boots or bleed air system. An electro-thermal heater is also adopted as a de-/anti-icing device since this device is easy to be installed for airplanes. However, these devices require electric energy to melt the accreted ice on surfaces of airplanes. Therefore, the optimization for the heating device is necessary to be investigated. In this study, we preform icing simulations of NACA0012 airfoil with the surface heating to investigate effects of the heating area on the ice accretion. The numerical procedure consists of four steps: generation of the computational grids; computation of the flow field around an airfoil; computation of the droplet trajectories to obtain the distribution of the impinged droplets; computation of the thermodynamics to obtain ice shapes. The compressible turbulent flow was assumed. The governing equations are two-dimensional continuity, Navier-Stokes, and energy equations. The Kato-Launder $k-\epsilon$ model was used as a turbulence model. The droplet trajectories were tracked in the Lagrangian approach. We made two assumptions: the droplets follow the flow field, while they do not affect the flow field; the force acting on droplets is only aerodynamic drag. For the thermodynamic calculation, an "extended Messinger model" was used to calculate the amount of ice. Although the model imposes the adiabatic condition on the surface of the airfoil, in the present study we modified this model to satisfy the Dirichlet condition (i.e., constant surface temperature). In order to clarify the effect of heating area, we have conducted icing simulations for different heating areas. From the results of the velocity field around the airfoil without heating, the thickness of the velocity boundary layer after icing became thicker than that before icing. On the other hand, due to the surface heating, the amount of icing and its area became small as increasing the heating area. The drag coefficient of the airfoil after icing with the heating is smaller than that without heating. Moreover, the drag coefficient decreases as increasing the heating area.

Multiscale Modeling of Plastic Deformation in Amorphous Solids

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ABSTRACT

Structurally disordered amorphous materials are noncrystalline solids that include metallic glasses, glassy polymers, amorphous ceramics, oxide glasses and so forth. Some of these glassy materials may exhibit plastic deformation. However, the exact mechanism of ductility in amorphous materials is still not completely understood, thus it is very difficult to predict the inelastic mechanical behaviors of amorphous materials at macroscale by using numerical methods, which usually require empirical modeling to represent the inelastic nature. Although multiscale models, which couples atomistic to macroscale scale, are expected to give us reliable modeling without using any empirical and experimental information, only few methods are available to the glassy materials due to their disordered and random microstructure. In this work, we have developed a hierarchical multiscale method to model the inelastic deformation in amorphous materials at macroscale without using any empirical or phenomenological constitutive modeling. The novelties of the multiscale method are three-fold: (1) the multiscale method employs an atomistic-based representative sampling cell (r-cell) obtained through statistical inferences of molecular statics modeling and simulation to obtain macroscale constitutive relations at continuum level; (2) The evolution of the r-cell provides precisely quantification of defect rearrangement in atomistic-scale, and hence the ramification on flow stress, and (3) it uses a special type of Cauchy-Born rules based on the Parrinello-Rahman molecular dynamics to construct an atomistic-informed finite element method. We coined the multiscale method as the coarse-grained Parrinello-Rahman (CG-PR) method. By doing so, we have successfully simulate plastic deformation in the Lennard-Jones binary glass (LJBG) at macroscale without using any empirical continuum level inelastic constitutive relations. For example, strain rate dependence of stress-strain relation is considered by using CG-PR. In addition, even hysteresis of stress-strain curve of cyclic deformation is spontaneously estimated, because rearrangement of atoms in r-cell represents variation of the plasticity. Moreover, we have shown that the CG-PR method can accurately capture the shear band formations in amorphous materials by using macroscale a single-notched thin plate model. The CG-PR simulation results on the shear band formations are compared with large-scale molecular dynamics simulations.

MODELLING OF THE DYNAMICS OF GRAB CRANES WITH A COMPLEX KINEMATIC STRUCTURE, TAKING INTO ACCOUNT THE LINKS' FLEXIBILITY AND ADVANCED FRICTION MODELS

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Abstract. A general mathematical model of a grab crane with a tree structure of a kinematic chain and the possibility of closed-loop subchains is presented in the paper. The formulated model takes into account the flexibility of the support system, links, drives and dry friction in joints. The joint coordinates and homogeneous transformation matrices, based on the Denavit-Hartenberg notation, are used to describe the motion of particular links. The equations of motion are derived using the Lagrange equations of the second kind. Flexible links are modelled using the rigid finite element method (RFEM). In this paper, the LuGre bristles' friction model is used. In numerical simulations, the grab crane consisting of a boom system forming an open-loop kinematic chain and two closed-loop subchains (formulated for hydraulic cylinders) is considered. The results of the calculations present an analysis of the influence of the friction and flexibility on the crane's dynamics.

NOMENCLATURE

$\alpha \in \{m_c, (s_c, 1), (s_c, 2)\}$ – indexes of main chain or subchains

g – acceleration of gravity

s – symbol of support

l – symbol of link

$rfe(\alpha, l, r)$ – symbol of r -th rigid finite element of link (α, l)

$sde(\alpha, l, s)$ – symbol of s -th spring-damping element of link (α, l)

$l^{(\alpha, l)}$ – length of link (α, l)

$m^{(\alpha, l)}$ – mass of link (α, l)

$\tilde{n}_{dof}^{(\alpha, l)}$ – number of generalised coordinates describing the motion of link (α, l)
with respect to the preceding link

$n_{dof}^{(\alpha, l)}$ – number of generalised coordinates describing the motion of link (α, l)
with respect to reference system $\{0\}$

- $n_{div}^{(\alpha,l)}$ – number of division of link (α,l)
 $n_{sde}^{(\alpha,l)}$ – number of sdes of link (α,l)
 $n_{rfe}^{(\alpha,l)}$ – number of rfes of link (α,l)
 $n_l^{(\alpha)}$ – number of links
 n_s – number of supports
 $s_\beta^{(sup,s)}, d_\beta^{(sup,s)} \Big|_{\beta \in \{x,y,z\}}$ – stiffness and damping coefficients of support s in β direction
 $s_\beta^{(\alpha,r)}, d_\beta^{(\alpha,r)} \Big|_{\beta \in \{\psi,\theta,\varphi\}}$ – stiffness and damping coefficients of rfe (α,l,r)
 $s_{dr}^{(\alpha,l)}, d_{dr}^{(\alpha,l)}$ – stiffness and damping coefficients of drive of link (α,l)
 $\tilde{~}^{(\alpha,l)}$ – vector of generalised coordinates describing the motion of link (α,l)
with respect to the preceding link, $\tilde{~}^{(\alpha,l)} = \left(\tilde{q}_i^{(\alpha,l)} \right)_{\substack{i=1,\dots,n_l^{(\alpha)} \\ i=1,\dots,\tilde{n}_{dof}^{(\alpha,l)}}}$
 $^{-}^{(\alpha,l)}$ – vector of generalised coordinates describing the motion of link (α,l)
with respect to the base system
 $^{(\alpha,l)}$ – vector of generalised coordinates describing the motion of link (α,l)
with respect to reference system $\{0\}$, $^{(\alpha,l)} = \left(q_i^{(\alpha,l)} \right)_{\substack{i=1,\dots,n_l^{(\alpha)} \\ i=1,\dots,\tilde{n}_{dof}^{(\alpha,l)}}}$
 $\mathbf{r}_A^{(\alpha,l)}$ – vector of position of point A defined in the local coordinate system of
link (α,l)
 $\mathbf{t}_{dr}^{(\alpha,l)}, \mathbf{f}_{dr}^{(\alpha,l)}$ – driving torque or force of link (α,l)
 $\mathbf{t}_f^{(\alpha,l)}, \mathbf{f}_f^{(\alpha,l)}$ – friction torque or force
 $\mathbf{H}^{(\alpha,l)}$ – pseudo-inertia matrix of link (α,l)
– reducing matrix, $= \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
 $\tilde{\mathbf{T}}^{(\alpha,l)}$ – homogeneous transformation matrix from the local coordinate system
of link (α,l) to the local reference system of the preceding link
 $\bar{\mathbf{T}}^{(\alpha,l)}$ – homogeneous transformation matrix from the local coordinate system
of link (α,l) to the base system
 $\mathbf{T}^{(\alpha,l)}$ – homogeneous transformation matrix from the local coordinate system
of link (α,l) to reference system $\{0\}$,
 $\mathbf{T}_i^{(\alpha,l)} = \frac{\partial \mathbf{T}^{(\alpha,l)}}{\partial q_i^{(\alpha,l)}}, \mathbf{T}_{ij}^{(\alpha,l)} = \frac{\partial^2 \mathbf{T}^{(\alpha,l)}}{\partial q_i^{(\alpha,l)} \partial q_j^{(\alpha,l)}}$

Friction parameters

- $\sigma_0^{(m_c)}, \sigma_1^{(m_c)}, \sigma_2^{(m_c)}$ – vectors of stiffness, damping and viscous friction coefficients of bristles, respectively
 $\delta^{(m_c)}$ – vector of deflections of bristles
 $\mu^{(m_c)}$ – vector of friction coefficients
 $\mu_s^{(m_c)}, \mu_k^{(m_c)}$ – vectors of static and kinetic friction coefficients, respectively
 $\dot{s}^{(m_c)}$ – vector of the Stribeck velocities

1 INTRODUCTION

For many years the control problems of handling equipment, including cranes, have been becoming more important. It is caused on the one hand by the desire to increase the efficiency of transshipment, on the other hand the care for the safety of service. The solution to these problems is to equip new constructions or to modify already existing ones by introducing measuring and executive systems. However, this approach can lead to significant increase in cost. Thanks to the use of computational methods in the area of simulation, the behavior of these devices in various operating conditions, it's possible to apply a strategy for the selection of appropriate control systems. For this purpose, dynamics models can be developed using commercial packages or using software dedicated to a specific construction. The developed mathematical models of grab cranes should take into account, e.g. the flexibility of the support system, links and drives. A significant influence on the dynamics response of the crane has also the friction phenomenon occurring in the joints.

The paper presents mathematical model of a grab crane¹⁻⁷ with a tree structure of a kinematic chain. This structure contains main chain (in the form of the open-loop kinematic chain) and two subchains (in the form closed-loop kinematic chains) which are models of hydraulic cylinders. The mathematical model takes into account the flexibility of the support system, links, drives and dry friction in joints^{6,7}. The clearance in joints is neglected. It is assumed, that the selected links of the crane are driven by torques or forces. These drives are modelled as flexible. The Denavit-Hartenberg notation based on the formalism of joint coordinates and homogeneous transformation matrices is used to describe kinematics of the grab crane⁸. The RFME is used to model the flexibility of links⁹. In this method, the rigid link is replaced by a system of rigid bodies interconnected by means of massless and dimensionless spring-damping elements. The main advantage of the RFEM is the ability to model flexible links using algorithms applied to the model of the rigid body systems with its small modification. Thanks to this, it is easy to use in computer implementation. The friction phenomenon is taken into account in all the joints of the main structure. The LuGre bristles' friction model is used to model this phenomenon¹⁰. This model allows to take into account the static and kinetic friction phases, and other effects like a preliminary displacement, the Stribeck effect and a frictional lag. The equations of motion are derived using the Lagrange equations of the second kind^{9,11}. These equations are supplemented by the Lagrange multipliers and constraint equations formulated for joints in which closed-loop kinematic chains are divided. The Baumgarte stabilization method is used for elimination of the constraint violation¹⁶.

The numerical calculations present the influence of the flexibility and friction in joints on the trajectory of the load and displacement of the crane's links.

2 MATHEMATICAL MODEL OF A GRAB CRANE WITH A FLEIBLE LINK

The grab crane consists of the main structure (m_c) in the form of open-loop kinematic chain (number of links $n_l^{(m_c)} = 8$) and two subchains ($(s_c,1), (s_c,2)$) in the form of closed-loop kinematic chains (number of links $\tilde{n}_l^{(\alpha)}|_{\alpha=\{(s_c,1), (s_c,2)\}} = 2$) (Fig. 1). The crane is connected to the ground by means of flexible supports ($n_s = 8$). The crane is driven by means of flexible drives in the form of torques ($\mathbf{t}_{dr}^{(m_c,2)}, \mathbf{t}_{dr}^{(m_c,8)}$) and forces ($\mathbf{f}_{dr}^{(m_c,4)}, \mathbf{f}_{dr}^{(s_c,1,2)}, \mathbf{f}_{dr}^{(s_c,2,2)}$). It is assumed the friction phenomenon occurs only in the joints of the main structure.

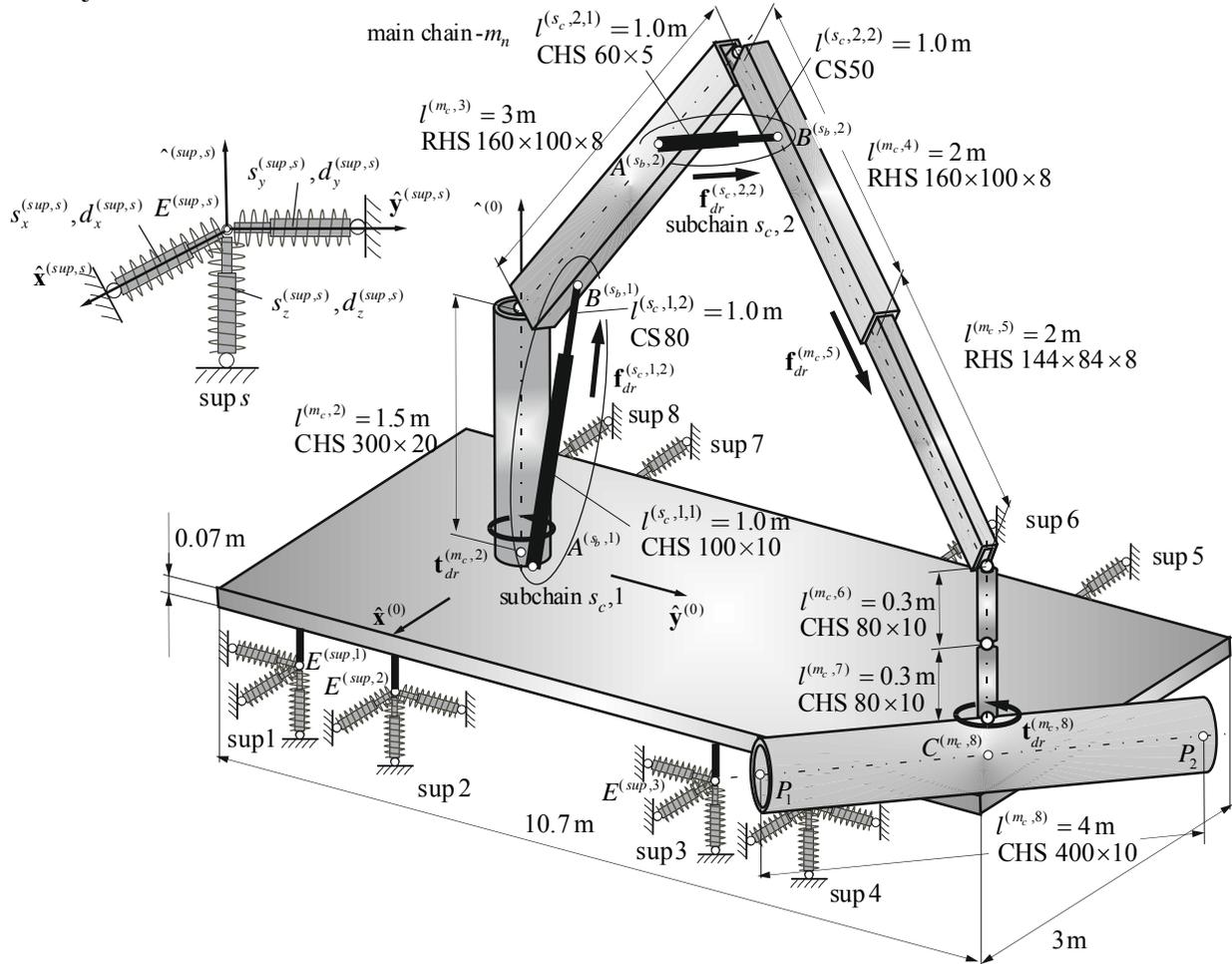


Fig. 1. Model of the grab crane

The joint coordinates together with the Denavit-Hartenberg notation, are used in order to describe the motion of particular links (Fig. 2). The RFEM is applied to discretise the flexible link. In this method, flexible link is replaced by the system of rigid elements (rfe) interconnected by means of spring-damping elements (sde).

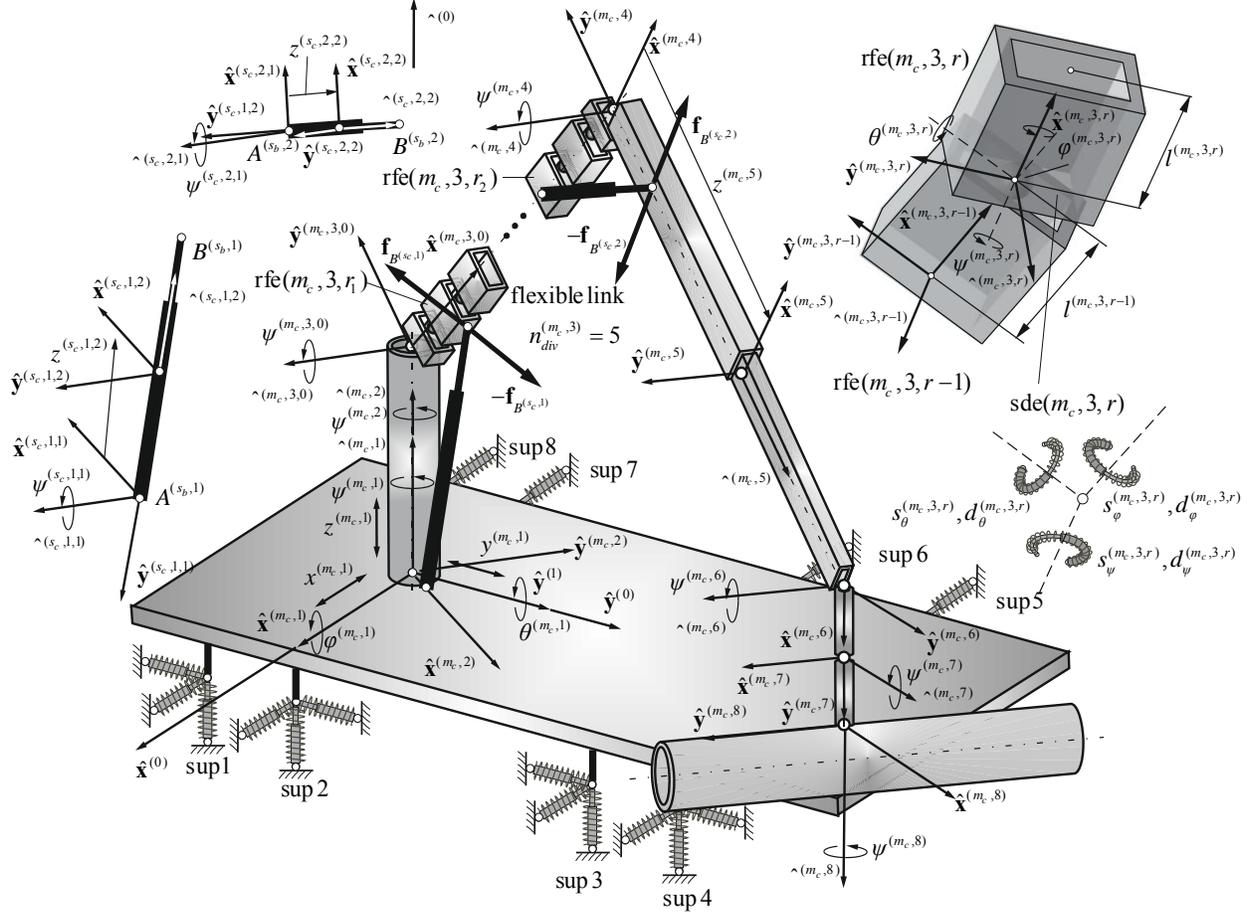


Fig.2. Denavit-Hartenberg notation

The motion of the grab crane is described by the vector of generalized coordinates:

$$= (q_i)_{i=1, \dots, n_{dof}} = \left[(m_c)^T \quad -(s_c,1)^T \quad -(s_c,2)^T \right]^T, \quad (1)$$

where:

- for main chain m_c

$$(m_c) = \left(q_i^{(m_c)} \right)_{i=1, \dots, n_{dof}^{(m_c)}} = \left[\sim(m_c,1)^T \quad \sim(m_c,2)^T \quad \sim(m_c,3)^T \quad \sim(m_c,4)^T \quad \sim(m_c,5)^T \quad \sim(m_c,6)^T \quad \sim(m_c,7)^T \quad \sim(m_c,8)^T \right]^T,$$

$$\sim(m_c,1) = \left[x^{(m_c,1)} \quad y^{(m_c,1)} \quad z^{(m_c,1)} \quad \psi^{(m_c,1)} \quad \theta^{(m_c,1)} \quad \varphi^{(m_c,1)} \right]^T,$$

$$\sim(m_c,2) = \left[\psi^{(m_c,2)} \right], \quad \sim(m_c,3) = \left[\sim(m_c,3,0)^T \quad \dots \quad \sim(m_c,3,r)^T \quad \dots \quad \sim(m_c,3,n_{dof}^{(m_c,3)})^T \right]^T,$$

$$\sim(m_c,3,0) = \left[\psi^{(m_c,3,0)} \right], \quad \sim(m_c,3,r) \Big|_{r=1, \dots, n_{dof}^{(m_c,3)}} = \left[\psi^{(m_c,3,r)} \quad \theta^{(m_c,3,r)} \quad \varphi^{(m_c,3,r)} \right]^T,$$

$$\sim(m_c,4) = \left[\psi^{(m_c,4)} \right], \quad \sim(m_c,5) = \left[z^{(m_c,5)} \right], \quad \sim(m_c,6) = \left[\psi^{(m_c,6)} \right], \quad \sim(m_c,7) = \left[\psi^{(m_c,7)} \right], \quad \sim(m_c,8) = \left[\psi^{(m_c,8)} \right],$$

- for subchain $(s_c,1)$

$$\begin{aligned}
(s_c,1) &= \left(q_i^{(s_c,1)} \right)_{i=1, \dots, n_{dof}^{(s_c,1)}} = \begin{bmatrix} \sim(m_c,1)^T & \sim(m_c,2)^T & \sim(s_c,1)^T \end{bmatrix}^T, \\
-(s_c,1) &= \left(\bar{q}_i^{(s_c,1)} \right)_{i=1, \dots, n_{dof}^{(s_c,1)}} = \begin{bmatrix} \sim(s_c,1,1)^T & \sim(s_c,1,2)^T \end{bmatrix}^T, \\
\sim(s_c,1,1) &= \left[\psi^{(s_c,1,1)} \right], \quad \sim(s_c,1,2) = \left[z^{(s_c,1,2)} \right],
\end{aligned}$$

- for subchain $(s_c,2)$

$$\begin{aligned}
(s_c,2) &= \left(q_i^{(s_c,2)} \right)_{i=1, \dots, n_{dof}^{(s_c,2)}} = \begin{bmatrix} \sim(m_c,1)^T & \sim(m_c,2)^T & \sim(m_c,3,0)^T & \dots & \sim(m_c,3,r_2)^T & \sim(s_c,2)^T \end{bmatrix}^T, \\
-(s_c,2) &= \left(\bar{q}_i^{(s_c,2)} \right)_{i=1, \dots, n_{dof}^{(s_c,2)}} = \begin{bmatrix} \sim(s_c,2,1)^T & \sim(s_c,2,2)^T \end{bmatrix}^T, \\
\sim(s_c,2,1) &= \left[\psi^{(s_c,2,1)} \right], \quad \sim(s_c,2,2) = \left[z^{(s_c,2,2)} \right].
\end{aligned}$$

The local homogeneous transformation matrices have the following forms:

-for main chain m_c

$$\begin{aligned}
\tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,1)} &= \begin{bmatrix} c\psi^{(b)}c\theta^{(b)} & c\psi^{(b)}s\theta^{(b)}s\varphi^{(b)} - s\psi^{(b)}c\varphi^{(b)} & c\psi^{(b)}s\theta^{(b)}c\varphi^{(a)} + s\psi^{(b)}s\varphi^{(b)} & x^{(b)} \\ s\psi^{(b)}c\theta^{(b)} & s\psi^{(b)}s\theta^{(b)}s\varphi^{(b)} + c\psi^{(b)}c\varphi^{(b)} & s\psi^{(b)}s\theta^{(b)}c\varphi^{(b)} - c\psi^{(b)}s\varphi^{(b)} & y^{(b)} \\ -s\theta^{(b)} & c\theta^{(b)}s\varphi^{(b)} & c\theta^{(b)}c\varphi^{(b)} & z^{(b)} \\ 0 & 0 & 0 & 1 \end{bmatrix}, \\
\tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,2)} &= \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & 0 \\ s\psi^{(b)} & c\psi^{(b)} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,3,0)} = \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & 0 \\ 0 & 0 & -1 & 0 \\ s\psi^{(b)} & c\psi^{(b)} & 0 & l^{(m_c,2)} \\ 0 & 0 & 0 & 1 \end{bmatrix}, \\
\tilde{\mathbf{T}}^{(b)} \Big|_{\substack{b=(m_c,3,r) \\ r=1, \dots, n_{dof}^{(m_c,3)}}} &= \begin{bmatrix} c\psi^{(b)}c\theta^{(b)} & c\psi^{(b)}s\theta^{(b)}s\varphi^{(b)} - s\psi^{(b)}c\varphi^{(b)} & c\psi^{(b)}s\theta^{(b)}c\varphi^{(b)} + s\psi^{(b)}s\varphi^{(b)} & l^{(m_c,3,r-1)} \\ s\psi^{(b)}c\theta^{(b)} & s\psi^{(b)}s\theta^{(b)}s\varphi^{(b)} + c\psi^{(b)}c\varphi^{(b)} & s\psi^{(b)}s\theta^{(b)}c\varphi^{(b)} - c\psi^{(b)}s\varphi^{(b)} & 0 \\ -s\theta^{(\alpha)} & c\theta^{(b)}s\varphi^{(b)} & c\theta^{(b)}c\varphi^{(b)} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \\
\tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,4)} &= \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & l^{(m_c,3,n_{dof}^{(m_c,3)})} \\ s\psi^{(b)} & c\psi^{(b)} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,5)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -z^{(b)} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \\
\tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,6)} &= \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -s\psi^{(b)} & -c\psi^{(b)} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,7)} = \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & l^{(m_c,6)} \\ 0 & 0 & 1 & 0 \\ -s\psi^{(b)} & -c\psi^{(b)} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},
\end{aligned}$$

$$\tilde{\mathbf{T}}^{(b)} \Big|_{b=(m_c,8)} = \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & 0 \\ 0 & 0 & 1 & l^{(m_c,7)} \\ -s\psi^{(b)} & -c\psi^{(b)} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

-for subchain $(s_c,1)$

$$\tilde{\mathbf{T}}^{(b)} \Big|_{b=(s_c,1,1)} = \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & x_{A^{(s_c,1)}}^{(m_c,2)} \\ 0 & 0 & -1 & y_{A^{(s_c,1)}}^{(m_c,2)} \\ s\psi^{(b)} & c\psi^{(b)} & 0 & z_{A^{(s_c,1)}}^{(m_c,2)} \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \tilde{\mathbf{T}}^{(b)} \Big|_{b=(s_c,1,2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -z^{(b)} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

-for subchain $(s_c,2)$

$$\tilde{\mathbf{T}}^{(b)} \Big|_{b=(s_c,2,1)} = \begin{bmatrix} c\psi^{(b)} & -s\psi^{(b)} & 0 & x_{A^{(s_c,2)}}^{(m_c,3,r)} \\ 0 & 0 & -1 & y_{A^{(s_c,2)}}^{(m_c,3,r)} \\ s\psi^{(b)} & c\psi^{(b)} & 0 & z_{A^{(s_c,2)}}^{(m_c,3,r)} \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \tilde{\mathbf{T}}^{(b)} \Big|_{b=(s_c,2,2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -z^{(b)} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$s\alpha^{(\beta)} = \sin\alpha^{(\beta)}, \quad c\alpha^{(\beta)} = \cos\alpha^{(\beta)}.$$

The transformation matrices to the global reference system are defined by following formulas:

$$\mathbf{T}^{(m_c,l)} \Big|_{l=1,\dots,\tilde{n}_l^{(m_c)}} = \mathbf{T}^{(m_c,l-1)} \tilde{\mathbf{T}}^{(m_c,l)}, \quad (2.1)$$

$$\mathbf{T}^{(s_c,1,l)} \Big|_{l=1,\dots,\tilde{n}_l^{(s_c,1)}} = \mathbf{T}^{(m_c,2)} \tilde{\mathbf{T}}^{(s_c,1,l)}, \quad (2.2)$$

$$\mathbf{T}^{(s_c,2,l)} \Big|_{l=1,\dots,\tilde{n}_l^{(s_c,2)}} = \mathbf{T}^{(m_c,3,r_2)} \tilde{\mathbf{T}}^{(s_c,1,l)}. \quad (2.3)$$

The equations of motion are derived using the Lagrange equations of the second kind. These equations are supplemented by constraint equations formulated for joints in which subchains are divided using the cut-joint technique.

The LuGre friction equations together with dynamics equations of motion can be written in following general form:

$$\dot{\cdot}^{(m_c)} = \mathbf{LuGre}(t, \cdot^{(m_c)}, {}^{(m_c)}), \quad (3.1)$$

$$\begin{bmatrix} \mathbf{M} & -\mathbf{C}^T \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\cdot} \\ \mathbf{f}_j \end{bmatrix} = \begin{bmatrix} \mathbf{e}(t, \cdot, \dot{\cdot}) - \mathbf{s}(\cdot, \dot{\cdot}) - \mathbf{d}(t, \cdot, \dot{\cdot}) - \mathbf{f}(t, {}^{(m_c)}, \dot{\cdot}^{(m_c)}) \\ \mathbf{c} \end{bmatrix}, \quad (3.2)$$

where:

$$(\mathbf{LuGre}_i)_{i=1,\dots,7} = \dot{q}_{n_i^{(1)}+i}^{(m_c)} \left(1 - \frac{\sigma_{0,i}^{(m_c)} z_i^{(m_c)} \operatorname{sgn}(\dot{q}_{n_i^{(1)}+i}^{(m_c)})}{\mu_{k,i}^{(m_c)} + (\mu_{s,i}^{(m_c)} - \mu_{k,i}^{(m_c)}) \exp\left(-\left(\frac{\dot{q}_{n_i^{(1)}+i}^{(m_c)}}{\dot{q}_{s,i}^{(m_c)}}\right)^2\right)} \right),$$

$$\boldsymbol{\mu}^{(m_c)} = \boldsymbol{\sigma}_0^{(m_c)} \mathbf{z}^{(m_c)} + \boldsymbol{\sigma}_1^{(m_c)} \dot{\mathbf{z}}^{(m_c)} + \boldsymbol{\sigma}_2^{(m_c)} \dot{\mathbf{q}}^{(m_c)},$$

$$\mathbf{M} = \sum_{\alpha \in \{m_c, (s_c,1), (s_c,2)\}} \mathbf{M}^{(\alpha)}, \quad \mathbf{f}_j = \begin{bmatrix} \mathbf{f}_{B^{(s_c,1)}} \\ \mathbf{f}_{B^{(s_c,2)}} \end{bmatrix},$$

$$\mathbf{M}^{(m_c)} = \begin{bmatrix} \mathbf{M}_{1,1}^{(m_c)} & \cdots & \mathbf{M}_{1,j}^{(m_c)} & \cdots & \mathbf{M}_{1,n_l}^{(m_c)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{M}_{i,1}^{(m_c)} & \cdots & \mathbf{M}_{i,j}^{(m_c)} & \cdots & \mathbf{M}_{i,n_l}^{(m_c)} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \mathbf{M}_{n_l}^{(m_c)},1} & \cdots & \mathbf{M}_{n_l}^{(m_c)},j} & \cdots & \mathbf{M}_{n_l}^{(m_c)},n_l} \end{bmatrix}, \quad \mathbf{M}^{(s_c,1)} = \begin{bmatrix} \mathbf{M}_{1,1}^{(s_c,1)} & \cdots & \mathbf{M}_{1,n_l}^{(s_c,1)} \\ \vdots & \ddots & \vdots \\ \mathbf{M}_{n_l}^{(s_c,1)},1} & \cdots & \mathbf{M}_{n_l}^{(s_c,1)},n_l} \end{bmatrix},$$

$$\mathbf{M}^{(s_c,2)} = \begin{bmatrix} \mathbf{M}_{1,1}^{(s_c,2)} & \cdots & \mathbf{M}_{1,n_l}^{(s_c,2)} \\ \vdots & \ddots & \vdots \\ \mathbf{M}_{n_l}^{(s_c,1)},1} & \cdots & \mathbf{M}_{n_l}^{(s_c,1)},n_l} \end{bmatrix},$$

$$\mathbf{M}_{i,j}^{(\alpha)} \Big|_{\alpha \in \{m_c, (s_c,1), (s_c,2)\}} = \sum_{l=\max\{i,j\}}^{n^{(\alpha)}} \mathbf{M}_{i,j}^{(\alpha,l)}, \quad \mathbf{M}_{i,j}^{(\alpha,l)} \Big|_{i,j=1,\dots,l} = \left(m_{n_{dof}^{(\alpha,i-1)} + m, n_{dof}^{(\alpha,j-1)} + n} \Big)_{\substack{m=1,\dots,\tilde{n}_{dof}^{(\alpha,i)} \\ n=1,\dots,\tilde{n}_{dof}^{(\alpha,j)}}},$$

$$m_{i,j}^{(\alpha,l)} = \operatorname{tr} \left\{ \mathbf{T}_i^{(\alpha,l)} \mathbf{H}^{(\alpha,l)} \left(\mathbf{T}_j^{(\alpha,l)} \right)^T \right\},$$

$$\mathbf{C} = \begin{bmatrix} \mathbf{C}_{B^{(s_c,1)}} \\ \mathbf{C}_{B^{(s_c,2)}} \end{bmatrix},$$

$$\mathbf{C}_{B^{(s_c,1)}} = \begin{bmatrix} \mathbf{C}_{1+\tilde{n}_{dof}^{(m_c,3,r_1)}}^{(m_c,3,r_1)} & -\mathbf{C}_{1+\tilde{n}_{dof}^{(s_c,1,2)}}^{(s_c,1,2)} \end{bmatrix}, \quad \mathbf{C}_{B^{(s_c,2)}} = \begin{bmatrix} \mathbf{C}_{1+\tilde{n}_{dof}^{(m_c,4)}}^{(m_c,4)} & -\mathbf{C}_{1+\tilde{n}_{dof}^{(s_c,2,2)}}^{(s_c,2,2)} \end{bmatrix},$$

$$\mathbf{C}^{(m_c,3,r_1)} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \begin{bmatrix} \bar{\mathbf{T}}_1^{(m_c,3,r_1)} \mathbf{r}_{B^{(s_c,1)}}^{(m_c,3,r_1)} & \cdots & \bar{\mathbf{T}}_{\tilde{n}_{dof}^{(m_c,3,r_1)}}^{(m_c,3,r_1)} \mathbf{r}_{B^{(s_c,1)}}^{(m_c,3,r_1)} \end{bmatrix},$$

$$\mathbf{C}^{(s_c,1,2)} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \begin{bmatrix} \bar{\mathbf{T}}_1^{(s_c,1,2)} \mathbf{r}_{B^{(s_c,1)}}^{(s_c,1,2)} & \cdots & \bar{\mathbf{T}}_{\tilde{n}_{dof}^{(s_c,1,2)}}^{(s_c,1,2)} \mathbf{r}_{B^{(s_c,1)}}^{(s_c,1,2)} \end{bmatrix},$$

$$\mathbf{C}^{(m_c,4)} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \begin{bmatrix} \bar{\mathbf{T}}_1^{(m_c,4)} \mathbf{r}_{B^{(s_c,2)}}^{(m_c,4)} & \cdots & \bar{\mathbf{T}}_{\tilde{n}_{dof}^{(m_c,4)}}^{(m_c,4)} \mathbf{r}_{B^{(s_c,2)}}^{(m_c,4)} \end{bmatrix}, \quad \mathbf{C}^{(s_c,2,2)} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \begin{bmatrix} \bar{\mathbf{T}}_1^{(s_c,2,2)} \mathbf{r}_{B^{(s_c,2)}}^{(s_c,2,2)} & \cdots & \bar{\mathbf{T}}_{\tilde{n}_{dof}^{(s_c,2,2)}}^{(s_c,2,2)} \mathbf{r}_{B^{(s_c,2)}}^{(s_c,2,2)} \end{bmatrix},$$

$$\mathbf{e} = \sum_{\alpha \in \{m_c, (s_c,1), (s_c,2)\}} \mathbf{e}^{(\alpha)},$$

$$\mathbf{e}^{(m_c)} = \begin{bmatrix} \mathbf{e}_1^{(m_c)} \\ \vdots \\ \mathbf{e}_i^{(m_c)} \\ \vdots \\ \mathbf{e}_{n_l^{(m_c)}}^{(m_c)} \end{bmatrix}, \mathbf{e}^{(s_c,1)} = \begin{bmatrix} \mathbf{e}_1^{(s_c,1)} \\ \vdots \\ \mathbf{e}_i^{(s_c,1)} \\ \vdots \\ \mathbf{e}_{n_l^{(s_c,1)}}^{(s_c,1)} \end{bmatrix}, \mathbf{e}^{(s_c,2)} = \begin{bmatrix} \mathbf{e}_1^{(s_c,2)} \\ \vdots \\ \mathbf{e}_i^{(s_c,2)} \\ \vdots \\ \mathbf{e}_{n_l^{(s_c,2)}}^{(s_c,2)} \end{bmatrix}, \mathbf{e}_i^{(a)} \Big|_{a \in \{m_c, (s_c,1), (s_c,2)\}} = - \sum_{l=i}^{n_l^{(a)}} \left(\mathbf{h}_i^{(a,l)} + \mathbf{e}_i^{(a,l)} \right),$$

$$\mathbf{h}_i^{(a,l)} \Big|_{i=1, \dots, l} = \left(h_{n_{dof}^{(a,j-1)} + k}^{(a,l)} \right)_{k=1, \dots, \tilde{n}_{dof}^{(a,i)}}, h_i^{(a,l)} = \sum_{m=1}^{n_{dof}^{(a,l)}} \sum_{n=1}^{n_{dof}^{(a,l)}} \text{tr} \left\{ \mathbf{T}_i^{(a,l)} \mathbf{H}^{(a,l)} \left(\mathbf{T}_{m,n}^{(a,l)} \right)^T \right\} \dot{q}_m^{(a,l)} \dot{q}_n^{(a,l)},$$

$$\mathbf{g}_i^{(a,l)} \Big|_{i=1, \dots, l} = \left(g_{n_{dof}^{(a,j-1)} + k}^{(a,l)} \right)_{k=1, \dots, \tilde{n}_{dof}^{(a,i)}}, \mathbf{g}_i^{(a,l)} = m^{(a,l)} \mathbf{g}_3 \mathbf{T}_i^{(a,l)} \mathbf{r}_{C^{(a,l)}}^{(a,l)},$$

$$\mathbf{s} = \sum_{\beta \in \{sup, sde\}} \mathbf{s}^{(\beta)},$$

$$\mathbf{s}^{(sup)} = \left[\mathbf{f}^{(sup)T} \right]^T, \mathbf{f}^{(sup)} = \sum_{s=1}^{n_s} \left(\left(\frac{\partial \mathbf{e}^{(sup,s)}}{\partial \tilde{z}^{(m_c,1)}} \right)^T \mathbf{S}^{(sup,s)} \mathbf{e}^{(sup,s)} + \left(\frac{\partial \dot{\mathbf{e}}^{(sup,s)}}{\partial \tilde{z}^{(m_c,1)}} \right)^T \mathbf{D}^{(sup,s)} \dot{\mathbf{e}}^{(sup,s)} \right),$$

$$\mathbf{e}^{(sup,s)} = \mathbf{T}^{(m_c,1)} \mathbf{r}_{E^{(sup,s)}}^{(m_c,1)},$$

$$\mathbf{S}^{(sup,s)} = \text{diag} \left\{ s_x^{(sup,s)}, s_y^{(sup,s)}, s_z^{(sup,s)} \right\}, \mathbf{D}^{(sup,s)} = \text{diag} \left\{ d_x^{(sup,s)}, d_y^{(sup,s)}, d_z^{(sup,s)} \right\},$$

$$\mathbf{s}^{(sde)} = \left[\mathbf{f}^{(sde)T} \right]^T, \mathbf{f}^{(sde)} = \mathbf{S}^{(m_c,3) \sim (m_c,3)}, \mathbf{S}^{(m_c,3)} = \text{diag} \left\{ 0, \mathbf{S}^{(m_c,3,1)}, \dots, \mathbf{S}^{(m_c,3,r)}, \dots, \mathbf{S}^{(m_c,3, n_{jfc}^{(m_c,3)})} \right\},$$

$$\mathbf{S}^{(m_c,3,r)} = \text{diag} \left\{ s_\psi^{(m_c,3,r)}, s_\theta^{(m_c,3,r)}, s_\phi^{(m_c,3,r)} \right\},$$

$$\mathbf{d} = \sum_{a \in \{m_c, (s_c,1), (s_c,2)\}} \mathbf{d}^{(a)}, \mathbf{d}^{(m_c)} = \begin{bmatrix} t_{dr}^{(m_c,2)} & f_{dr}^{(m_c,5)} & t_{dr}^{(m_c,8)} \end{bmatrix}^T, \mathbf{d}^{(s_c,1)} = \begin{bmatrix} f_{dr}^{(s_c,1,2)} \end{bmatrix}^T,$$

$$\mathbf{d}^{(s_c,2)} = \begin{bmatrix} f_{dr}^{(s_c,2,2)} \end{bmatrix}^T, t_{dr}^{(m_c,i)} \Big|_{i \in \{2,8\}} = - \left[s_{dr}^{(m_c,i)} \left(\psi_{dr}^{(m_c,i)} - \psi^{(m_c,i)} \right) + d_{dr}^{(m_c,i)} \left(\dot{\psi}_{dr}^{(m_c,i)} - \dot{\psi}^{(m_c,i)} \right) \right],$$

$$f_{dr}^{(a)} \Big|_{a \in \{(m_c,5), (s_c,1,2), (s_c,2,2)\}} = \left[s_{dr}^{(a)} \left(z_{dr}^{(a)} - z^{(a)} \right) + d_{dr}^{(a)} \left(\dot{z}_{dr}^{(a)} - \dot{z}^{(a)} \right) \right],$$

$$q_{dr}^{(a)} = \begin{cases} q_{int}^{(a)} + 10 \frac{q_{inc}^{(a)}}{T^3} t^3 - 15 \frac{q_{inc}^{(a)}}{T^4} t^4 + 6 \frac{q_{inc}^{(a)}}{T^5} t^5 & \text{for } t < T \\ q_{fin}^{(a)} & \text{for } t \geq T \end{cases}, q_{inc}^{(a)} = q_{fin}^{(a)} - q_{int}^{(a)},$$

$$\mathbf{f} = \begin{bmatrix} t_f^{(m_c,2)} & t_f^{(m_c,3)} & t_f^{(m_c,4)} & f_f^{(m_c,5)} & t_f^{(m_c,6)} & t_f^{(m_c,7)} & t_f^{(m_c,8)} \end{bmatrix}^T,$$

$$\mathbf{c} = \begin{bmatrix} \mathbf{c}_{B^{(s_c,1)}} \\ \mathbf{c}_{B^{(s_c,2)}} \end{bmatrix},$$

$$\mathbf{c}^{(s_c,1)} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \left[\left(\sum_{i,j=1}^{\tilde{n}_l^{(s_c,1,2)}} \bar{\mathbf{T}}_{i,j}^{(s_c,1,2)} \dot{q}_i^{(s_c,1,2)} \dot{q}_j^{(s_c,1,2)} \right) \mathbf{r}_{B^{(s_c,1)}}^{(s_c,1,2)} - \left(\sum_{i,j=1}^{\tilde{n}_l^{(m_c,3,r)}} \bar{\mathbf{T}}_{i,j}^{(m_c,3,r)} \dot{q}_i^{(m_c,3,r)} \dot{q}_j^{(m_c,3,r)} \right) \mathbf{r}_{B^{(s_c,1)}}^{(m_c,3,r)} \right],$$

$$\mathbf{c}^{(s_c,2)} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \left[\left(\sum_{i,j=1}^{\tilde{n}_l^{(s_c,2,2)}} \bar{\mathbf{T}}_{i,j}^{(s_c,2,2)} \dot{q}_i^{(s_c,2,2)} \dot{q}_j^{(s_c,2,2)} \right) \mathbf{r}_{B^{(s_c,2)}}^{(s_c,2,2)} - \left(\sum_{i,j=1}^{\tilde{n}_l^{(m_c,4)}} \bar{\mathbf{T}}_{i,j}^{(m_c,4)} \dot{q}_i^{(m_c,4)} \dot{q}_j^{(m_c,4)} \right) \mathbf{r}_{B^{(s_c,2)}}^{(m_c,4)} \right].$$

The dynamics of the grab crane forms the set of differential-algebraic equations with index 1. The constraint violations at the position and velocity level are eliminated by using the Baumgarte stabilization method.

3 SIMULATION RESULTS

For the assumed initial configuration of the crane the statics task is solved using the Newton-Raphson iterative method. Values of the joint coordinates obtained from this task take into account the influence of the deformation of flexible supports, links and drives due to the effects of gravity. The dynamics equations of motion and state equations, are integrated using the Runge-Kutta method of the fourth order with a constant step size. In each the integration step, the Newton-Euler recursive algorithm is applied to determine the joint forces and torques. These forces and torques are necessary to determine friction torques acting in rotational joints and friction forces acting in prismatic joints.

The parameters of the crane supports, drives and friction are presented in Tabs. 1-3, respectively.

Table 1: Parameters of the crane supports

sup s	1	2	3	4	5	6	7	8
$\mathbf{r}_{E^{(sup,s)}}^{(m_c,1)} [\text{m}]$	$\begin{bmatrix} 1.5 \\ 0 \\ -0.57 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1.5 \\ 1.0 \\ -0.57 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1.5 \\ 8.0 \\ -0.57 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1.5 \\ 9.0 \\ -0.57 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -1.5 \\ 9.0 \\ -0.57 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -1.5 \\ 8.0 \\ -0.57 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1.5 \\ 1.0 \\ -0.57 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -1.5 \\ 0 \\ -0.57 \\ 0 \end{bmatrix}$
$\mathbf{S}^{(sup,s)} [\text{Nm}^{-1}]$	$\text{diag}\{3 \cdot 10^6, 3 \cdot 10^6, 1 \cdot 10^7\}$							
$\mathbf{D}^{(sup,s)} [\text{Ns m}^{-1}]$	$\text{diag}\{5 \cdot 10^4, 5 \cdot 10^4, 9 \cdot 10^4\}$							

Table 3: Drive parameters

drive	$(m_c, 2)$	$(s_c, 1, 2)$	$(s_c, 2, 2)$	$(m_c, 5)$	$(m_c, 8)$
$q_{int}^{(\alpha)} [\text{deg}, \text{m}]$	0	1.9	0.55	1.0	270
$q_{fin}^{(\alpha)} [\text{deg}, \text{m}]$	90	1.9	0.75	0.7	270
$s_{dr}^{(\alpha)} [\text{Nradm}^{-1}, \text{Nm}^{-1}]$	10^7	10^8	10^8	10^8	10^7
$d_{dr}^{(\alpha)} [\text{Nsradm}^{-1}, \text{Nsm}^{-1}]$	$7 \cdot 10^3$				

Table 3: Friction parameters

joint j	2	3	4	5	6	7	8
$\boldsymbol{\mu}_s^{(m_c)}$	$[0.2 \ 0.2 \ 0.2 \ 0.2 \ 0.2 \ 0.2 \ 0.2]$						
$\boldsymbol{\mu}_k^{(m_c)}$	$[0.1 \ 0.1 \ 0.1 \ 0.1 \ 0.1 \ 0.1 \ 0.1]$						
$\boldsymbol{\sigma}_0^{(m_c)} [\text{rad}^{-1}, \text{m}^{-1}]$	$[10^2 \ 10^2 \ 10^2 \ 10^3 \ 10^2 \ 10^2 \ 10^2]$						
$\boldsymbol{\sigma}_1^{(m_c)} [\text{srad}^{-1}, \text{s m}^{-1}]$	$[10 \ 10 \ 10 \ 10^{3/2} \ 10 \ 10 \ 10]$						
$\boldsymbol{\sigma}_2^{(m_c)} [\text{srad}^{-1}, \text{s m}^{-1}]$	$[10 \ 10 \ 10 \ 10^{3/2} \ 10 \ 10 \ 10]$						
$\dot{s}^{(m_c)} [\text{rads}^{-1}, \text{ms}^{-1}]$	$[1.75 \cdot 10^{-2}$	$1.75 \cdot 10^{-2}$	$1.75 \cdot 10^{-2}$	0.001	$1.75 \cdot 10^{-2}$	$1.75 \cdot 10^{-2}$	$1.75 \cdot 10^{-2}]$

The influence of the flexibility of link 3 and friction in the joints on the trajectories of selected points of load in $\hat{\mathbf{x}}^{(0)}\hat{\mathbf{y}}^{(0)}$ plane are presented in Fig. 3, whereas courses of $z_{\alpha}^{(0)}|_{\alpha=\{P_1, C^{(m_c, 8)}, P_2\}}$ components are shown in Fig. 4. The courses of the driving forces in the actuators are presented in Fig. 5.

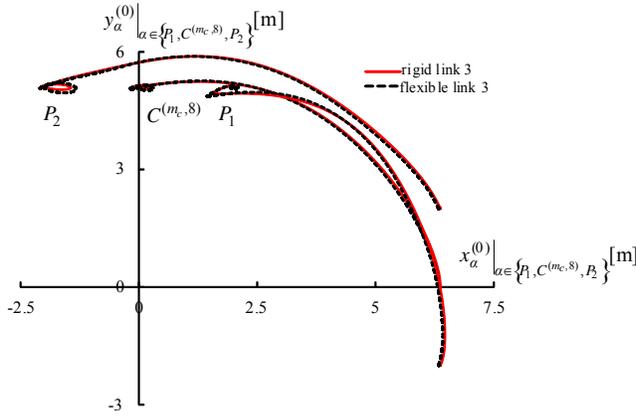


Fig. 3. Trajectories of selected points of the load

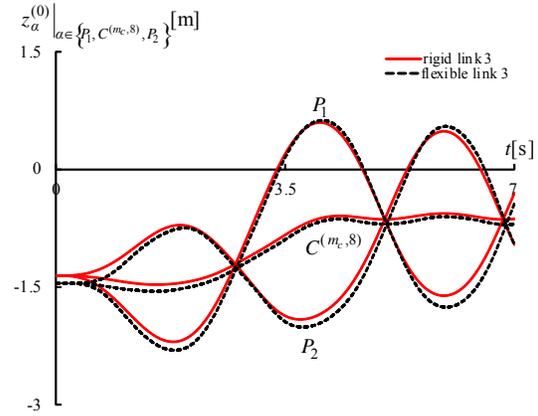


Fig. 4. Time courses of the z component

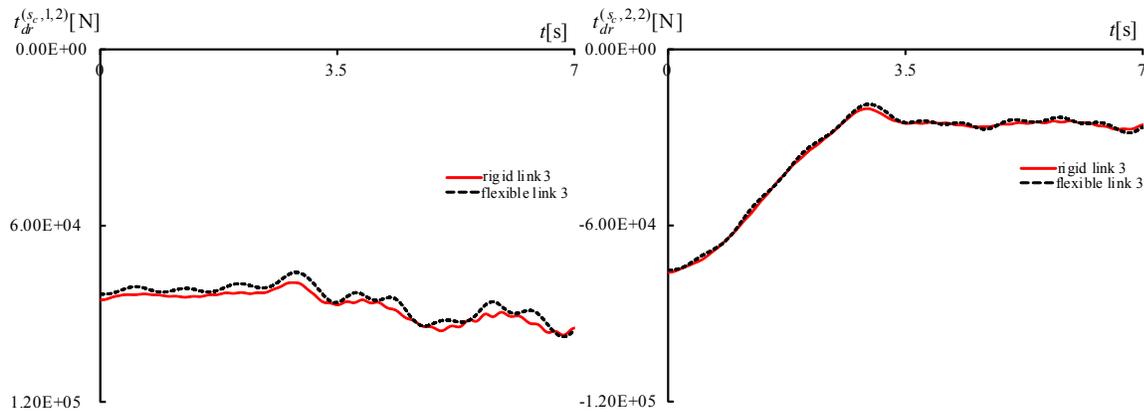


Fig. 5. Time courses of the driving forces

The performed calculations show that considered phenomena of the modeled crane have a influence on the crane dynamics. The flexibility introduce some oscillations in the time courses of the actuator driving function. These oscillations can arise when smaller actuators' stiffness values are taken in calculations.

4 CONCLUSIONS

The mathematical model of the grab crane presented in this paper has been used to analyse the influence of flexibility (supports, links and drives) and friction on crane's dynamics. The joint coordinates and homogeneous transformation matrices have been applied to describe the geometry of the grab crane. The dynamics equations of motion have been derived using the formalism of the Lagrange equations of the second kind. The RFEM has been used to discretize the flexible link. The LuGre bristles' friction model has been applied to model the friction in joints. The phenomena taken into account in the mathematical model of grab crane have the significant influence on

behavior of the handling load, and in the authors' opinion the presented results can be useful while a process of designing.

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On the Implications of Hyperparameters Choices in Bayesian Inference of Random Fields

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ABSTRACT

Inverse problems occur whenever one aims to infer information about a physical system based on observations. If the uncertain model parameters are expressed in terms of random fields, the complexity of the inverse problem is increased as uncertain parameters of random functions need to be identified, which generally renders the problem high-dimensional. We formulate the inference problem probabilistically using a Bayesian approach. A challenge in Bayesian inference with random fields is the definition of the prior distribution for the autocovariance kernel of the field. In practice, the prior knowledge is typically not sufficient to favor a particular kernel. One alternative is to define a hierarchical Bayesian model by decomposing the prior information about the autocovariance kernel into one or more conditional distributions of uncertain hyperparameters. In this paper, we employ the Karhunen-Loève expansion to represent the random field. The influence of different probabilistic modeling strategies for the hyperparameters, such as the truncation order of the expansion and the correlation length of the field, is investigated. We provide insight into the selection of prior probability distributions for the hyperparameters. We further analyze the computational implications of the adopted hierarchical Bayesian approach. The study is exemplarily performed on a structural beam with spatially variable flexibility.

Towards Support and Neutral Data Exchange for Isogeometric Analysis (IGA) in the ISO 10303 Standard

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ABSTRACT

Isogeometric Analysis (IGA) is a computational analysis methodology that offers the possibility of integrating Finite Element Analysis (FEA) into conventional design tools, bridging the chasm between the current industrial verticals of Computer-Aided Design (CAD) and Computer-Aided Engineering (CAE). Although the benefits of IGA are vast and numerous as an engineering technology, one key problem is that conventional file formats limit the ability to share IGA modeling data between users. Currently users are forced to create their own file formats, rely on academic researchers' personal implementations, or use specific CAx application formats for the translation and storage of IGA data, often compromising the users' design intent. Support in current interchange formats, such as STEP, is limited as the standards were developed around conventional CAD and CAE, classically separated technologies prior to the invention of IGA. This has severely hindered both the potential for collaboration between users as well as the more critical objective: large-scale commercial adoption of IGA as an industrial technology. ISO 10303 plays an indispensable role as the de facto neutral file format in the world of CAD-CAE data exchange and has recently adopted critically important IGA features such as locally refined splines (e.g., T-splines, LR-splines, etc.), trivariate (volumetric) spline representations, etc. [1,2]. While these additions greatly increase the ability of IGA designers and analysts, it does not allow for the ability to exchange common unstructured mesh representations frequently encountered in industrial models, containing extraordinary points (E.P.s) of arbitrary valence. As part of its Digital Thread for Smart Manufacturing Project [3], The National Institute of Standards and Technology's (NIST) Engineering Laboratory (EL) has taken an active role in resolving the IGA data exchange problem. These activities have shed new insights on integrated CAx model representations in a IGA-centric view where CAD-CAE model definition is simultaneous. [1] T. Dokken, V. Skytt, J. Haenisch, K. Bengtsson, Isogeometric Representation and Analysis: Bridging the Gap Between CAD and Analysis, in: 47th AIAA Aerosp. Sci. Meet. New Horiz. Forum Aerosp. Expo., American Institute of Aeronautics and Astronautics, n.d. doi:10.2514/6.2009-1172. [2] V. Skytt, J. Haenisch, Extension of ISO 10303 with Isogeometric Model Capabilities, (2013). [3] Digital Thread for Smart Manufacturing, NIST. (2014). <https://www.nist.gov/programs-projects/digital-thread-smart-manufacturing>.

Experimental Verifications for Indirect Bridge Frequency Measurement

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ABSTRACT

According to the idea of indirect bridge frequency measurement proposed by Yang and co-workers [1-3], a moving test vehicle can be regarded as a message receiver to detect vibration data of the bridge that it passed. In the present study, an experimental setup will be carried out for indirect frequency measurement of a simply supported beam using a passing test vehicle with the feature of adjustable frequencies. The test vehicle is design as a single-degree-of-freedom unit in vertical vibration and guided by a set of tensile strings in self-equilibrium state so that it can drive the vehicle to move along the beam axis with full contact. To remain the test vehicle running over the beam at constant speed, this study proposed a set of cantilever spiral spring devices to adjust the frequency by regulating the arch length of the spiral springs. From the present experimental results, the indirect bridge inspection method is applicable to frequency monitoring of a bridge. Moreover, the harder stiffness adjusted by the spiral spring device can give a more accurate prediction for measuring bridge frequencies than the softer one. References [1] Yang, Y. B., Lin, C. W., and Yau, J. D., Extracting bridge frequencies from the dynamic response of a passing vehicle, *J. Sound & Vibr.*, 272(3-5), 2004, 471-493. [2]Lin, C. W., and Yang, Y. B., Use of a passing vehicle to scan the bridge frequencies - an experimental verification, *Eng. Struct.*, 27(13), 2005, 1865-1878. [3]Yang, Y. B., Li, Y.C., and Chang, K.C., Constructing the mode shapes of a bridge from a passing vehicle: a theoretical study, *Smart Structures & Systems, An Int. J.*, 13(5), 2014, 797-819.

Numerical and Physical Modeling of Stringer Stiffened Silo Collapse Subject to Eccentric Discharge Flow

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ABSTRACT

Stringer stiffened metal silos for grain and other bulk material storage are highly efficient structures designed to sustain axially symmetric loads. Accidental operation of eccentric outlets while the silo is loaded at full capacity might induce eccentric discharge flows under which severe non-symmetric loads develop onto the silo outer shell. These loads, being far from the structure design conditions, can cause localized buckling of the stringer stiffeners, loss of structural stability and, ultimately, its collapse. In this work both physical and numerical modeling of the interaction between granular flow and structural dynamic response are developed and compared for concentric and eccentric flow conditions. Small scale structured models of stringer stiffened silos, were assembled using aluminum foil for the outer shell and dried pasta straws for the vertical stringer stiffeners, while sand is used to model the granular flow. Thus, a complete structured small scale model with individual stringer stiffeners was developed with this approach. Experiments were performed varying the outlet positions, from concentric to mild (37%) and severe (74%) eccentric. Small to negligible deformations of the scale model were observed for concentric and mild eccentric flow conditions, while progressive individual stringer stiffeners buckling and full collapse of the structure was observed for severe eccentric flows. A numerical model of the structural dynamic response was implemented following Ivanov [1] proposal for a structural-DEM method. Shell elements were connected together with elongation, bending and torsional springs, modeling both the outer shell and the vertical stringer stiffeners. Full geometrical non-linearity and inertial behaviour is fully captured intrinsically by the DEM method. Load due to grain flow was modeled after Sadowski [2]. Numerical experiments again show small to negligible deformations for concentric flow conditions. Mildly eccentric flow produced limited localized deformations of the structure, with no buckling of the individual stringer stiffeners. Meanwhile, for severe eccentric flow, deep localized buckling, in the shape of 'smile' buckles, was observed followed by complete loss of structural stability and full collapse. Comprehensive physical and numerical modeling of structural behaviour of stringer stiffened silos was accomplished in this work, with novel approaches to the implementation of both physical models with individual stringer stiffeners and numerical modeling through a structural-DEM method.

Uncertainties in Geotechnical Laboratory Tests and Centrifuge Experiments

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ABSTRACT

Geomaterials are essentially inhomogeneous. Although a lot of their constitutive models have been proposed and some have been used in practice, numerical models considering inhomogeneity and uncertainties have not established. Centrifuge modelling is one of the most popular and reliable physical modelling for geomaterials; therefore the results of centrifuge experiments have been used for validation process of newly developed numerical method including constitutive models of soil. The material parameters of constitutive models have been calibrated with laboratory tests such as triaxial compression tests. However, uncertainties in the laboratory tests and the centrifuge experiments have not been considered in most validation cases of geotechnical problems although it was well known that geotechnical centrifuge modeling includes some uncertainties such as inhomogeneity of model ground and soil structures, unrepeatability of external loading. In this study many cases with the same target experimental conditions were performed through triaxial tests and centrifuge experiments for shear and consolidation behaviors of clay ground. The uncertainties in the deformation of clay ground were discussed.

Micromechanical Modeling and Simulation of Ductile Failure under Combined Tension and Shear

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ABSTRACT

The Gurson (1977) model of ductile failure by void growth to coalescence is widely used in the structural integrity assessment of engineering components. Recent work has focused on addressing some well-known limitations of the Gurson model such as the inability to predict fracture at low stress triaxialities, incorporating the dependence of yield criterion on the Lode parameter, and the effect of “void coalescence” or plastic flow localization at the mesoscale of the voids. Recently, Keralavarma (2017) proposed a multi-surface plasticity model for a porous isotropic material by combining the Gurson void growth model with the void coalescence model of Keralavarma and Chockalingam (2016). Here, the theoretical framework of the multi-surface model is revisited and the model predictions are calibrated with micromechanical finite element simulations of void growth using the unit cell model. An initially cubic unit cell with a concentric spherical void is deformed to failure under a combination of triaxial tensile and shear loads. Periodic boundary conditions are used and the stresses are applied proportionally such that the macroscopic stress triaxiality, T , and lode parameter, L , remain constant throughout the loading history. The average stress-strain response, the evolution of porosity and the macroscopic strain at the onset of coalescence obtained from the simulations are compared with predictions from the multisurface model for a wide range values of T and L . It is shown that the effective response predicted by the multi-surface model is in good quantitative agreement with the cell model simulations for materials with low strain hardening capacity. The triaxiality and Lode parameter dependence of the strain to failure is correctly predicted by the model. For materials with high strain hardening capacity, the model is shown to significantly underestimate the ductility, especially under shear dominated loading conditions. A phenomenological extension of the model, motivated by the theory of strain localization in elasto-plastic materials, is shown to significantly improve the model predictions for hardening materials. References 1. Gurson, A.L. , 1977. Continuum theory of ductile rupture by void nucleation and growth: part i—yield criteria and flow rules for porous ductile media. *J. Eng. Mat. Tech.* 99, 2–15. 2. Keralavarma, S.M. , 2017. A multi-surface plasticity model for ductile fracture simulations. *J. Mech. Phys. Solids*, 103:100-120. 3. Keralavarma, S.M. , Chockalingam, S. , 2016. A criterion for void coalescence in anisotropic ductile materials. *Int. J. Plast.* 82, 159–176.

One-dimensional Fluid Model of In Vivo Pulmonary Arterial Hemodynamic Data

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ABSTRACT

Pulmonary arterial hypertension (PAH) is a severe disease of the pulmonary vasculature that is characterized by high blood pressure in the lungs. During the development of PAH, the pulmonary vasculature undergoes structural remodeling that compromises its normal physiological function. Here, we investigate how the changes in wall mechanics contribute to the pulmonary vascular hemodynamics in PAH using a 1D fluid model. Using Euler equations and assuming an axisymmetric blood flow in the pulmonary arteries, the deformation of the arterial wall is prescribed using linear elasticity [1]. The initial-boundary value problem is initialized using in-vivo measurements of blood flow and pressure from the main pulmonary artery (MPA) at the inlet ((first node) to predict pressure and cross-sectional area propagation along the vessel length. Blood pressure, flow, outer diameter, wall thickness and in-situ length of the MPA are measurements from normo- and hypertensive male rats taken during open chest surgery. The pressure-area relation is a linearization of the thin shell model around the area value at no pressure [2]. The elastic modulus is the average of the right and left pulmonary artery elastic modulus measured under tubular biaxial tensile tests [3] immediately after hemodynamic measurements. In the current numerical scheme, no boundary conditions at the outlet are imposed. The system of equations was discretized in time and space, and was solved using Euler's method in MATLAB. Pressure and elastic modulus increased with the progression of PAH, but flow remained overall constant. By using these data, the model was able to predict pressure that closely resembles to that measured pressure at the inlet of the MPA. After three cardiac cycles, a slight decrease in the peak flow, pressure and cross-sectional area was observed. This could be interpreted as the attenuation of the waveform due to the buffering effect of the vessel. The computed dynamic cross-section area is about 26% higher than the measured value at zero stress during opening-angle experiments. When testing how the elastic modulus of one animal on another, we found the pressure and flow waveforms to remain unaffected. However, area predictions were amplified indicating the model being sensitive to wall stiffness. Boundary conditions will be investigated to determine how the changes in the wall mechanics influence the hemodynamics of the vasculature in PAH. [1] P Lee, et al. Biomech. Model. Mechanobiol., 2016. [2] MS Olufsen, Am. J. Physiol., 1999. [3] ER Pursell, et al. J. Biomech. Eng., 2016.

An Alternative Computational Approach to Evaluate the Directional Behavior of Periodic Media

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ABSTRACT

One of the most relevant problems in the dynamic analysis of periodic media is the determination of the directional behavior of the material. As a result, the preferred propagation directions, which are a function of the material structure, are identified. In the typical analysis method one computes the material dispersion surfaces which result after solving a generalized eigenvalue problem corresponding to the imposition of the so-called Bloch periodic boundary conditions upon the unit cell. The preferred propagation directions are identified from the shapes appearing in the iso-frequency contour plots of the gradients over the first two modes of the dispersion surfaces. As a complement, it is also frequent to use a polar histogram of these gradients. This approach has a conceptual inconvenience. First, in the dispersion relations, the wave types and modes are usually mixed. For instance, it may be the case that information from several wave types originated at different Brillouin zones appear in the first mode. Similarly, since the approach is based on the first two modes the analysis might erroneously eliminate directional behavior associated to the high frequency regime. In this work we present an alternative approach to conduct directional analysis of periodic media where we consider the first N modes from the generalized eigenvalue problem. We compute the magnitude and directional distribution of a single vector field V computed after considering the N modes simultaneously. The results are then presented as a combination of phase velocity and a vector count held over V . Since we take information from several modes, as opposed to single mode biased methods, we obtain more representative descriptions of the directional response valid in the low and high frequency regime. Our presentation is organized as follows: - Description of the classical approach for directional analysis focusing on its two major drawbacks. - Detailed description of the proposed approach using N modes and a vector field. - Applications showing the validity and versatility of the proposed approach.

Direct Simulation of Granular Collapses Using $\mu(I)$ -like Rheology

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ABSTRACT

We introduce an accurate numerical method for the computation of 2D and 3D granular collapse under gravity flows using different versions of the $\mu(I)$ rheology. We use a time-dependent regularization algorithm to solve the model using a finite element method, combined with anisotropic mesh adaptation to capture accurately the quasi-static vs. inertial flow zones, and using a variational multiscale method. A Level-Set method, based on self-reinitialization of the signed distance function, aims to capture and follow efficiently the interface between the fluid/air domains. We show that this rheology can capture the two experimentally observed types of spreading and the corresponding scaling laws, both in 2D and 3D collapses. Sensitivity analysis on rheological constants was performed for quasi-static and inertial parameters, in order to verify the universality (no dependency on grain type) of flow features such as relative spreading vs. aspect ratio, and normalized distance-time. We also demonstrate the effect of additional lengthscales on the dynamics of spreading, not discussed in previous literature.

A First Order System Discontinuous Petrov-Galerkin Method Using Continuous Trial Spaces

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ABSTRACT

We present a new type discontinuous Petrov-Galerkin (DPG) method for finite element (FE) approximations of boundary value problems of second order linear partial differential equations (PDEs) in the spirit of the DPG method introduced by Demkowicz and Gopalakrishnan [1, 2]. The new DPG method uses a first order system weak representation of the governing PDEs, and distinguishes itself by using classical C_0 or continuous function spaces for the trial functions, in an effort to reduce computational cost. Discontinuous function spaces, however, are employed for the test functions and therefore the test functions can be solved locally at the element level by using the DPG philosophy in [1, 2]. Hence, they are optimal in the sense that they guarantee inherently stable FE approximations with best approximation properties in terms of the energy norm. The local contributions of test functions can be numerically solved on each element with high numerical accuracy and do not require the solution of global variational statements. 2D numerical verifications and convergence studies are to be presented for the solution of second order partial differential equations, including convection dominated convection-diffusion problems with highly oscillatory (diffusion) coefficients. [1] L. Demkowicz and J. Gopalakrishnan. Analysis of the DPG method for the Poisson equation. *SIAM Journal on Numerical Analysis*, 49(5):1788–1809, 2011. [2] L. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov-Galerkin methods. II. Optimal test functions. *Numerical Methods for Partial Differential Equations*, 27(1):70–105, 2011.

Atomic-Microscale Modeling of Phonons in the Molecular Crystal RDX Using Accurate Phonon Lifetimes

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ABSTRACT

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. Additionally, for the first time, we also calculate phonon lifetimes in RDX throughout the first Brillouin zone. This is accomplished by running lattice dynamics and molecular dynamics simulations and then fitting the mode projected spectral energy density. The use of mode specific lifetimes significantly increases the accuracy of the thermal conductivity values predicted with Boltzmann transport equation calculations, allowing for an additional source of anisotropy to appear in the thermal conductivity tensor. Our tabulation of mode specific lifetimes contains fine grained details about energy transport in RDX which may be of interest to those researching shock induced initiation and multiphonon up-pumping in RDX. 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.

DIMENSION ADAPTIVE PSEUDO-SPECTRAL PROJECTION FOR A PERMANENT SYNCHRONOUS MOTOR WITH UNCERTAIN PARAMETERS

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Key words: Polynomial Chaos Expansion, Electrical Drives, Error Control, Uncertainty Quantification, Sparse Grids, Surrogate Modeling.

Summary. Many industrial problems are based on simulation models which require knowledge on parameter values. In practice, however, exact information is rarely available. For example, variations in component tolerances due to manufacturing processes may translate to parameter uncertainties influencing the outcome of simulation models. This makes uncertainty quantification crucial to establish the reliability of simulation results. Using the classical "Monte Carlo method" type design of experiment would randomly sample in parameter space, perform simulations for each sample and afterwards combine the results to estimate all statistical quantities of interest. The main drawback of this method is that usually many samples, i.e. many simulations, are required to reach a satisfactory error level in the statistical predictions (thousands to hundreds of thousands samples). In contrast, Polynomial Chaos Expansions (PCEs) are popular spectral surrogate models typically applied to solve uncertainty propagation problems. They quantify the effect of statistical fluctuations in simulation model outputs due to uncertainty in parameter space using orthogonal polynomials. Various techniques exist to compute the coefficients of PCEs. A canonical way is to approximate the coefficients by numerical quadrature, evaluate the simulation model at the quadrature nodes and post-process the results. However, this approach suffers from aliasing errors, which can be circumvented by tailoring the PCE to the numerical quadrature (in our case a "Smolyak sparse grid") in a special way. This gives rise to the so-called "Pseudo-Spectral Projection method" (PSP), which we consider in a dimension adaptive version (aPSP). The major advantage of aPSP is its automatic error control, which provides a robust error estimation on all adaptive iterations, and hence allows an estimation on the quality of each design of experiment. In this work, we investigate a PMSM (permanent magnet synchronous motor) with uncertain geometrical and physical parameters, for example the positioning of magnets. Our focus

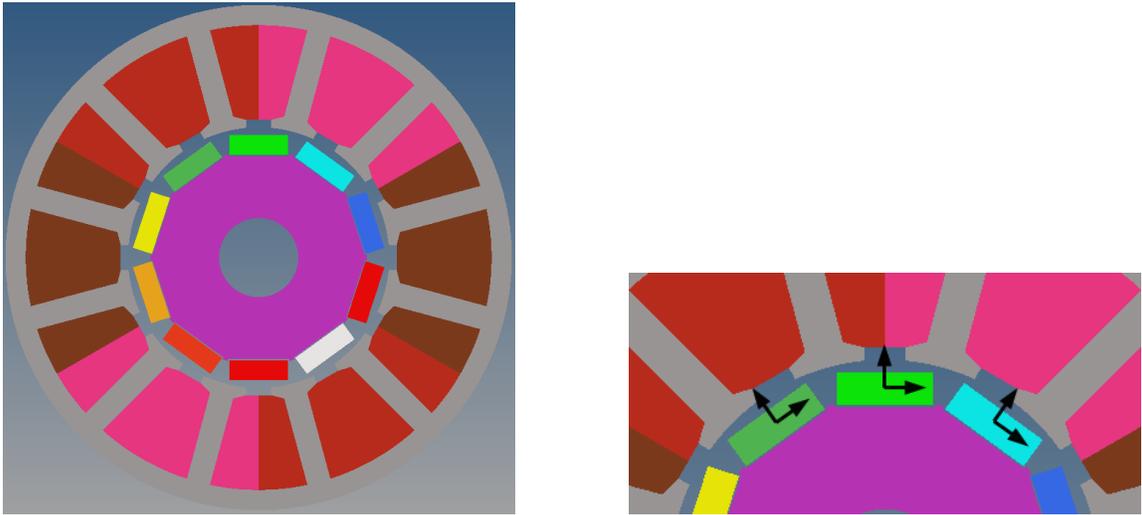
is on analyzing the convergence behavior of aPSP on different quantities of interest, such as the cogging torque, and their post-processing via Fast-Fourier-Transform. We measure convergence via the error estimation of aPSP and compare it to the convergence of root-mean-square errors, which is computed by point-wise squared differences of surrogate model evaluations and a test data set.

1 INTRODUCTION

With regard to the development of the fuel prices and the world-wide CO_2 discussion the trend to electrification in motor vehicles is unbroken. More and more vehicles are equipped with e.g. electromotive supported steering systems, brake systems and the trend to electric mopeds (eScooter) and electromotive driven bicycles (eBikes) continues world-wide. The rising demand of electrical drives asks for designs with more power density, which are cheaper and more durable. Such solutions can be reached only with the most modern development methods. The main goal in the development of electric motors is to guarantee the demanded functions with minimal costs. The costs of an electrical machine consist not only of the material and the production costs, but also contain the costs by scrap during manufacturing. To minimize this scrap, it has to be guaranteed that the characteristics of the motor keep to the demanded limits under influence of manufacturing tolerances and noise factors. A motor design which fulfills this demand is called "robust". To evaluate the robustness of a motor design, classic approaches like Monte Carlo analysis or Latin Hypercube Sampling (LHS) could be used. Unfortunately these approaches suffer from a very high number of samples. If the computation time is high, e.g. due to the usage of finite element methods, the number of samples has to be reduced significantly. This need is even more important, when the robustness analysis has to be performed within a multi-objective optimization for each single design, see [7]. In this paper, the cogging torque of a permanent magnet synchronous surface-magnet motor is investigated, see Section 2. For this type of motor, the no-load torque is significantly disturbed by magnet tolerances, e.g. position and magnetic remanence and new orders appear in the spectrum of the torque signal. To assess how these tolerances affect the cogging torque, a dimension-adaptive pseudo spectral projection method (aPSP) is applied to a two-dimensional (spatial) magneto-static finite-element model to compute the stochastic cogging torque waveform along with the stochastic torque spectrum, see Section 3. In Section 4 the simulation results are compared with results achieved by a LHS method taken as reference to validate the aPSP method. The iteration dependent global error computed by the aPSP method is also documented to illustrate the method efficiency. Finally, a sensitivity analysis is performed on the stochastic cogging torque waveform obtained by the aPSP method to experience which parameters are dominating.

2 INVESTIGATED MOTOR

The presented methodology is used to analyze the cogging torque of a permanent magnet synchronous machine with 10 rotor poles and 12 stator teeth (see Fig. 1a). Here the cogging torque signal (no load torque), which is known to be sensitive to geometrical and material disturbances, is analyzed. We analyze the torque signal using a Fourier decomposition. In the nominal motor, without any disturbance, the cogging torque signal consists of only the order 60, the least common multiplier of the rotor poles and stator tooth, and multiples of it. Any disturbance in the rotor can affect these orders and, in case of asymmetrical disturbances, will also lead to the appearance of additional orders with the number of stator teeth and multiples (i.e. 12, 24, 36, ...), see [4]. Fig. 2a respectively 2b shows the cogging torque waveform respectively the related Fourier spectrum of a disturbed motor. In this paper, three magnets are chosen to be disturbed with 3 uncertain parameters each. The uncertain parameters of each magnet are: its position deviation in radial and tangential direction (see Fig. 1b) and its magnetic remanence. The parameters are assumed to be uniformly distributed within the interval [-1;1].



(a) Sketch of a permanent magnet synchronous machine with 10 rotor poles and 12 stator teeth.

(b) Uncertain positioning of three magnets.

Figure 1: Sketch of motor magnet alignment. The positioning of three magnets is uncertain along the sketched directions. In addition, the value for the remanence of each of those magnets is also uncertain.

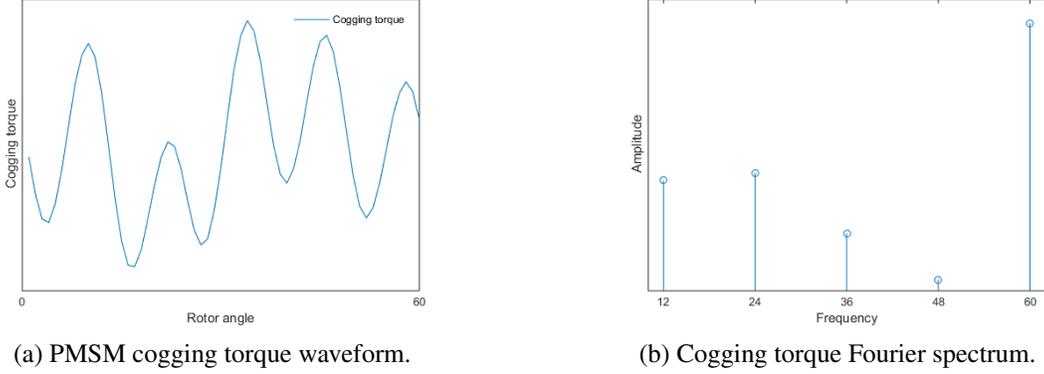


Figure 2: PMSM cogging torque waveform and related Fourier spectrum.

3 DIMENSION ADAPTIVE PSEUDO SPECTRAL PROJECTION

Mathematically speaking, the problem formulation as described in Section 2 is a forward uncertainty propagation task. The variation of the position of the three magnets and their corresponding remanence is modeled using 9 independent, uniformly distributed random variables denoted by $\xi = (\xi_1, \dots, \xi_9)$. We employ the generalized Polynomial Chaos expansion (PCE) [8, 3] to model the dependence of the cogging torque, denoted by Tq on the parameter vector ξ , i.e.,

$$Tq = Tq(\xi) = \sum_{i=0}^{\infty} Tq_i \psi_i(\xi). \quad (1)$$

Here, $\{\psi_i\}_{i=0}^{\infty}$ denote multivariate polynomials, which are orthogonal with respect to the Uniform probability density of the random vector ξ , i.e. each ψ_i is a multivariate Legendre polynomial. Two tasks remain: first, the infinite series in (1) must be truncated to become feasible for computation and second, the coefficients Tq_i must be computed numerically for all $i \in \mathbb{N}$ remaining in the truncated series. Afterwards, the PCE can be used in post-processing as a surrogate for the original simulation model to compute all relevant statistical information of Tq (mean, variance, probability density, sensitivity information, ...). Notably, there exist analytical expressions for the mean, the variance and the Sobol indices used in global sensitivity analysis, e.g. $\mathbb{E}(Tq) = Tq_0$ is the mean and $\sigma^2(Tq) = \sum_{i=1}^{\infty} Tq_i^2$ is the variance (if the polynomials are normalized with respect to the L^2 norm).

3.1 Truncation of the Polynomial Chaos expansion

In its standard formulation, the total polynomial degree of the PCE gets cut at some specified order $p \in \mathbb{N}$, which yields the approximated PCE:

$$Tq(\xi) \approx \sum_{i=0}^P Tq_i \psi_i(\xi). \quad (2)$$

The number of terms $P + 1$ is analytically determined via:

$$P + 1 = \frac{(p + M)!}{p!M!},$$

where $M \in \mathbb{N}$ denotes the number of uncertain parameters, i.e. in our case $M = 9$. After truncation, the coefficients Tq_i , $i = 0, \dots, P$ can be approximated by multivariate numerical quadrature - the so-called "non-intrusive spectral projection":

$$Tq_i(\xi) \approx \int Tq(\eta) \psi_i(\eta) w(\eta) d\eta = \sum_{j=1}^N w_j Tq(\xi^j) \psi_i(\xi^j), \quad i = 0, \dots, P, \quad (3)$$

where w denotes the joint probability density function of ξ , w_j and ξ^j denote the weights and nodes of the employed numerical quadrature rule of size N . However, when M increases the number of quadrature nodes required to keep a high accuracy grows exponentially. Often sparse grids [6] are employed to mitigate this so-called "curse of dimensionality". However, the approximation of the PCE coefficients by numerical quadrature suffers from aliasing errors due to a loss of discrete orthogonality if higher order polynomials are used in the truncated PCE [2, 1]. To overcome this drawback the PCE truncation can be tailored to the quadrature nodes of the sparse grid. It is based on applying the Smolyak algorithm used for construction of the sparse grid directly to the PCE system in (1). The method is then called "Pseudo-Spectral Projection" (see following section).

3.2 Pseudo-spectral projection

The PCE as defined in (1) uses a single enumeration index. It can be equivalently defined using a multi-index notation:

$$Tq(\xi) = \sum_{\alpha \in \mathbb{N}^M} Tq_\alpha \psi_\alpha(\xi), \quad (4)$$

where $\alpha = (\alpha_1, \dots, \alpha_M) \in \mathbb{N}^M$ is the multi-index, and $\psi_\alpha(\xi) := \prod_{i=1}^M \psi_{\alpha_i}^i(\xi_i)$. Here, $\psi_{\alpha_i}^i$ denote the univariate Legendre polynomial of degree α_i , which only depend on ξ_i ,

respectively. The multi-index notation has the advantage, that the truncation of the PCE can be defined in a more generic way:

$$Tq(\xi) \approx \sum_{\alpha \in \mathcal{I}} Tq_{\alpha} \psi_{\alpha}(\xi), \quad (5)$$

where $\mathcal{I} \subset \mathbb{N}^M$ denotes the index set used for truncation. There exists a one-to-one correspondence between the single and multi-index notation. For example, setting $\mathcal{I} = \{\alpha \in \mathbb{N}^M : \sum_{i=1}^M \alpha_i \leq p\}$ by enumeration one obtains the truncation specified in (2) for a given total order $p \in \mathbb{N}$.

The construction of sparse grids is based on Smolyak's algorithm. It can be applied directly to numerical quadrature rules and thereby it generates a set of sparse quadrature nodes and weights. In the Pseudo-Spectral Projection method, Smolyak's algorithm is applied to the polynomial basis of the PCE. The procedure is outlined in the following.

For each dimension $i = 1, \dots, M$ and polynomial degree $n \in \mathbb{N}$ we first define the projection operators \mathcal{P}_n^i by:

$$\mathcal{P}_n^i(Tq) := \sum_{j=0}^n Tq_j \psi_j^i, \quad (6)$$

with Tq_j , $j = 0, \dots, n$ defined as in (3). Then for each $i = 1, \dots, M$ define the one-dimensional hierarchical surplus operator by:

$$\begin{aligned} \Delta_{m(p)}^i &:= \mathcal{P}_{m(p)}^i - \mathcal{P}_{m(p-1)}^i, \quad p \geq 1, \\ \Delta_0^i &:= 0, \end{aligned}$$

where $m : \mathbb{N} \rightarrow \mathbb{N}$, $m(0) := 0$ is strictly increasing and called the "growth rule". Common choices for m are:

$$\begin{aligned} m(p) &:= p, \\ m(p) &:= 2p - 1, \quad m(0) := 0 \\ m(p) &:= 2^p - 1. \end{aligned}$$

For a given multi-index $k = (k_1, \dots, k_M)$ the multi-dimensional hierarchical surplus operator Δ_k is then defined by:

$$\Delta_k := \Delta_{m(k_1)}^1 \otimes \dots \otimes \Delta_{m(k_M)}^M. \quad (7)$$

Finally, Tq is approximated via:

$$Tq \approx \sum_{k \in \mathcal{I}} \Delta_k. \quad (8)$$

3.3 Error control and dimension adaptivity

The hierarchical surplus defined in (7) is used to define an error estimator ϵ_k^2 for each multi-index $k \in \mathcal{I}$:

$$\epsilon_k^2 := \|\Delta_k\|^2. \quad (9)$$

The norm $\|\cdot\|$ is typically chosen as the L^2 norm of the probability space of ξ . Having an error estimator, the remaining question is how to appropriately define the truncation index set \mathcal{I} . To this end, the dimension-adaptive sparse grid algorithm of Gerstner and Griebel [5, 1] can be easily adapted to the pseudo-spectral projection. It iteratively constructs the set \mathcal{I} based on the errors estimated by ϵ_k . Thereby, $\mathcal{I} := \mathcal{A} \cup \mathcal{O}$, with \mathcal{A} and \mathcal{O} denoting the so-called "active" (candidate set for further refinement) and "old" index sets, respectively. The overall error of the algorithm is measured using the global error

$$\epsilon := \sqrt{\sum_{k \in \mathcal{A}} \epsilon_k^2}. \quad (10)$$

It terminates when either the error falls below some threshold or some maximum number of iterations is achieved. The resulting method is then called "dimension adaptive Pseudo-Spectral Projection (aPSP)".

4 NUMERICAL RESULTS

In this section, the aPSP method is first applied to compute the stochastic cogging torque waveform. After computing the surrogate model with aPSP, the waveform is sampled using plain-vanilla Monte Carlo sampling to investigate the stochastic torque spectrum. All results are compared to reference results obtained by Latin Hypercube Sampling (LHS) of the original forward model. In addition, a global sensitivity analysis based on the "Analysis of Variance / Sobol indices" is performed on the waveform from the validated aPSP surrogate to identify dominant parameters.

4.1 Stochastic cogging torque waveform

The stochastic cogging torque waveforms computed by both LHS and aPSP methods (iteration 1 using 19 runs and iteration 7 using 103 runs) are shown in Fig. 3. The first aPSP iteration (only 19 runs required) is already capable to match the results computed with the LHS method very well. Increasing the iteration number, we observe a further convergence of the approximation error.

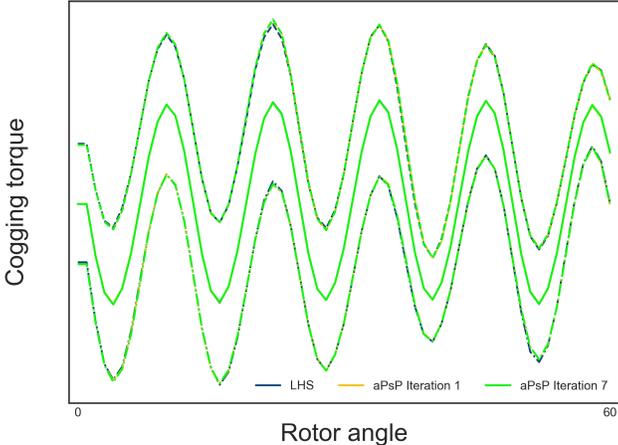


Figure 3: Stochastic cogging torque waveforms (average and 5% – 95% extrem quantiles).

4.2 Stochastic cogging torque spectrum

The stochastic cogging torque spectra computed by both LHS and aPSP methods are shown in Fig. 4.

The stochastic spectrum computed with the aPSP surrogate matches the one computed with the LHS method very well after a few iterations only (only 103 runs required).

4.3 Global error and sensitivity

The iteration dependent global error (see Section 3) during the stochastic cogging torque waveform computation is shown in Fig. 5a. The error decreases monotonically, yet in our belief its value overestimates the true error of the surrogate. We verified this statement by computing a root-mean square error (RMSE) relatively to the cogging torque waveform with respect to the LHS test data set, see Fig. 5b. The RMSE for the final iteration is of order 10^{-1} . The reason for the slow convergence of the global error is due to the strongly varying global sensitivity of the parameters as a function of the rotation angle, see Fig. 5c.

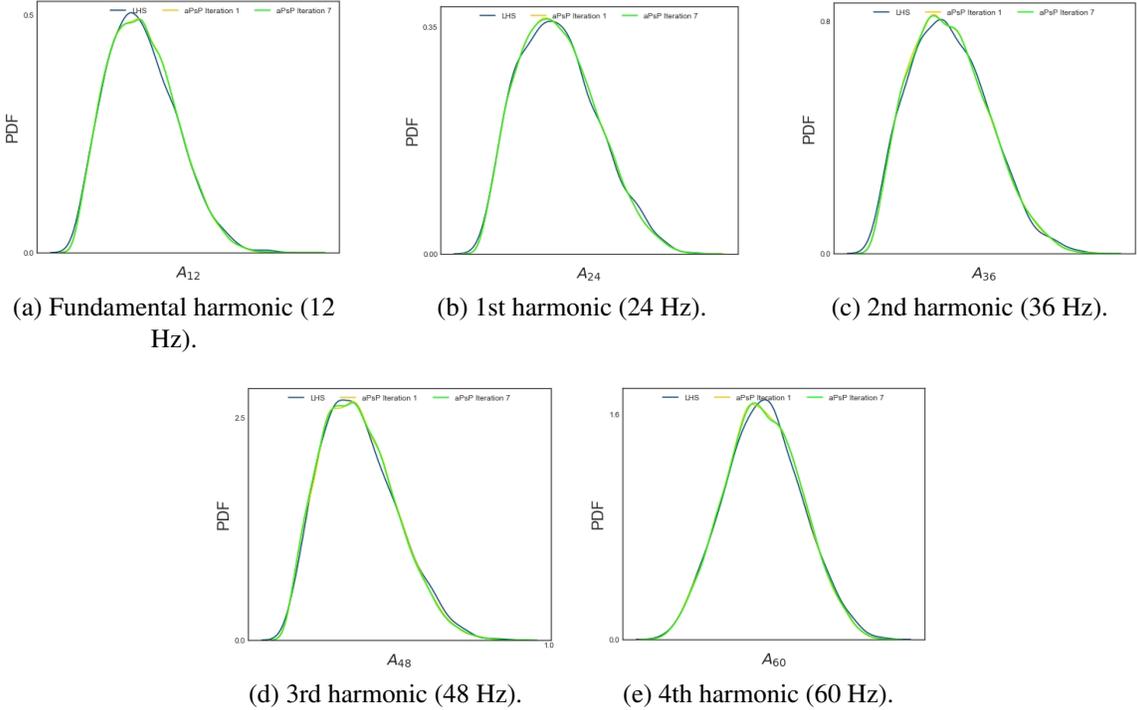
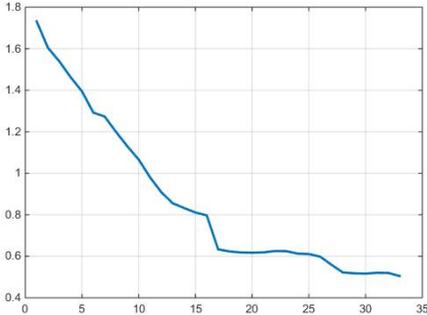


Figure 4: Cogging torque stochastic harmonic analysis.

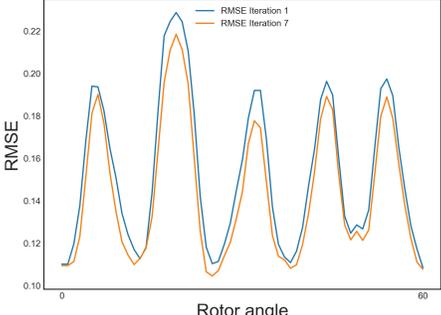
5 CONCLUSIONS

In this work we applied the dimension adaptive Pseudo-Spectral Projection method (aPSP) to a PSM with 9 uncertain parameters. The main difficulty is to obtain a forward uncertainty analysis of the PSM with high accuracy but using only a few model evaluations (due to the high computational cost associated with the solution of the forward model). The dimension adaptivity addresses this problem from two sides: the number of samples is kept low by only selecting "important" samples in the parameter space and a surrogate model (the Polynomia Chaos expansion) for which the aPSP provides an error estimator. To analyze the convergence behavior of the error estimator, we also compared the results to a reference obtained by Latin Hypercube Sampling applied to the original forward model.

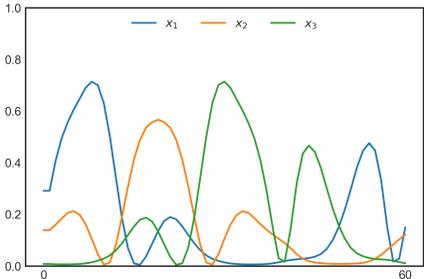
The numerical results demonstrate that the error estimation of the aPSP is slightly pessimistic but the reference data is matched very well using only few forward model evaluations. However, as the rotor's position is changed, the Sobol indices of the parameters also change in value making unimportant parameters more important and vice versa. This causes the error of the aPSP to decrease only slowly, since it is unclear how the rotor an-



(a) Global error vs. iteration number.



(b) RMSE vs. rotor position.



(c) Global sensitivity of parameters.

Figure 5: Convergence and sensitivity obtained by the aPSP method.

gle should be appropriately treated within the aPSP. We used averaging over the angle to obtain only scalar quantities, but in principle other choices may perform differently.

Our current research is on evaluating different strategies to deal with the angle dependency and in addition to apply the aPSP to a larger set of uncertain parameters in the PSM.

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The Origin of Tensile-compressive Asymmetry in Amorphous and Semicrystalline Polymers

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ABSTRACT

The mechanical properties of polymeric materials strongly depend on their morphology and spatial arrangements. Polymeric materials also exhibit asymmetric yield strength and strain hardening in tension and compression. We examine the microscopic origin of this asymmetry for amorphous and semicrystalline polymers by performing large-scale molecular dynamics simulations. We compute the tensile and compressive response of amorphous and semicrystalline polymers of a semiflexible bead-spring polymer model [1] for various chain lengths [1,2,3]. Investigating the microstructural evolution of polymers, we find that the asymmetry arises from a different arrangement of polymers during tensile and compressive deformation. In tension, the chains align themselves along the tensile axis that leads to a net global nematic ordering of the chains end-to-end vectors. During compression, the polymers arrange themselves in a plane perpendicular to the compressive axis and as a result a novel anti-nematic ordering of the chains end-to-end vectors emerges. Computing ratio of microscopic stretch of the polymers relative to the macroscopic stretch, we find that the semicrystalline polymers deform less affinely than their amorphous counterparts. Interestingly, the degree of non-affinity is smaller during compression. [1] H. Meyer and F. Muller-Plathe, J. Chem. Phys. 115, 7807 (2001). [2] S. Jabbari-Farouji, J. Rottler, M. Perez, O. Lame, A. Makke & J.-L. Barrat, Physical Review Letters 118 (21), 217802 (2017) [3] S. Jabbari-Farouji and D. Vandembroucq in preparation

Shear Banding and Finite Size Effects in a Mesoscopic Model of Amorphous Composites

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ABSTRACT

We study the plastic behavior of amorphous media reinforced by hard particles using a mesoscopic depinning-like lattice model. In this model, lattice sites represent coarse-grained shear transformations which interact via an Eshelby elastic interaction kernel. Hard inclusions are assigned larger yield thresholds than sites associated to the amorphous matrix. Results show a complex size dependence of the effective flow stress of the amorphous composite: one associated to the amorphous matrix and another one associated to the hard inclusions. While the former results in an $1/N$ dependence of the flow stress with the system size, the latter predicts a size dependent threshold concentration below which no reinforcement is observed. We show that the threshold concentrations correspond to the percolation of shear bands through the system in between the hard inclusions. Above the threshold concentration no shear bands can percolate without breaking through a hard site. In this regime we find that the distance of the flow stress to a linear mixing law scales as $(\log N/N)^{1/2}$ and the flow stress increases with the system size. The linear mixing law then gives an upper bound to the flow stress. We find that the increase in the flow stress is associated to the breakthrough of the weakest shear band over hard sites and the flow stress value is governed by the accumulation of plastic activity along the weakest band. We develop a simple model based on the weakest shear band hypothesis: although a simple linear mixing law is unable to predict the flow stress when applied to the bulk, we find that it works surprisingly well when applied to the weakest shear band. Our model turns out to predict well the flow stress value, its size dependence and even the flow stress fluctuations. [1] B. Tyukodi, C. Lemarchand, J. Hansen, D. Vandembroucq, "Finite size effects in a model for plasticity of amorphous composites", Physical Review E, 93, 023004 (2016) [2] B. Tyukodi, S. Patinet, D. Vandembroucq, S. Roux, "From depinning transition to plastic yielding of amorphous media: A soft-modes perspective", Physical Review E, 93, 063005 (2016)

Amorphous Plasticity from Atomic Scale to Mesoscopic Scale

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ABSTRACT

In crystalline materials, plasticity results from the motion of defects of the crystalline lattice, dislocations. The absence of structural order in glasses requires to look for alternative microscopic mechanisms for the plastic deformation. A common hypothesis consists in considering series of localized rearrangements of the amorphous structure : Shear Transformations. In this talk we review recent results obtained for the characterization of such Shear Transformations at the atomic scale. We first present a recent numerical method allowing to characterize local yield thresholds in model 2D lennard-Jones glasses prepared by molecular dynamics. We discuss their connection to the plastic activity observed upon shearing and their dependence on the protocol of preparation of the glass. In particular we give quantitative evidence that the more relaxed the glass, the higher the local plastic thresholds. We also discuss the tensorial character of the Shear Transformations. We then present recent results obtained with lattice models of amorphous plasticity at a mesoscopic scale and discuss first attempts of coarse-graining the plastic behavior of glasses from atomic scale to mesoscopic scale. References : S. Patinet et al. Connecting Local Yield Stresses with Plastic Activity in Amorphous Solids, Phys. Rev. Lett. 117, 045501 (2016) A. Barbot et al. Local yield stress statistics in model amorphous solids, submitted to Phys. Rev. E B. Tyukodi et al. From depinning transition to plastic yielding of amorphous media: A soft-modes perspective, Phys Rev. E 93, 063005 (2016)

Numerical Treatment of Boundary Layers for High-Order DG Schemes by Using Basis Enrichment

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ABSTRACT

Large Eddy Simulations (LES) of moderate and high Reynolds number flows becomes exceedingly expensive, if turbulent structures in the boundary layer have to be resolved. Several techniques for wall-modeled LES exist to model the near-wall turbulence and momentum transfer. The novel Extended Discontinuous Galerkin scheme (XDG) takes a priori properties of the expected form of the solution into account to resolve steep gradients. The underlying Discontinuous Galerkin (DG) scheme have gained a significant role in high-order spatial discretization techniques in computational sciences in the last decade. Some of the reasons for its steady growing popularity are the high order accuracy with geometrical flexibility, allowing adaptivity as well as easy parallelization based on the compact stencil. The main idea of the XDG approach is to extend the standard polynomial solution space of the Discontinuous Galerkin method by an appropriate enrichment function representing an approximate analytical solution of the flow, which cannot be resolved by the polynomials. In this way the solution is not prescribed, but the numerical method has the possibility to choose the appropriate solution out of the given function space via the Galerkin projection. In the application for turbulent boundary layer, we can make use of the universal properties of the mean velocity distribution in order to resolve the velocity gradients in the near-wall region with very coarse meshes. Several methods using an extended problem-tailored solution space such as the partition-of-unity method (PUM) or the extended finite element method (XFEM) have been developed. They are applied for approximation of solutions with jumps, singularities and other locally non-smooth features arising in cracks, solidification, shocks etc. Within the presentation, first the theoretical background of the XDG scheme is presented based on the discretization techniques of the DG method. With regard to turbulent boundary layers, the Singular Perturbation Problem for the linear scalar advection diffusion equation as well as for the non linear inviscid Burgers' equation in one dimension are considered in order to evaluate the ideas of basis enrichment numerically in the case of high gradients, which can not be represented by polynomials. In conclusion the application of XDG for the compressible Navier-Stokes equations to a turbulent channel flow in Implicit LES is shown with very coarse meshes.

Simulation of Blast Effects in Monumental Structures

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ABSTRACT

Highly representative monuments are unfortunately too often the objective of destructions and the threats on them increase in the present situation. Research on the effects of an explosion inside monuments are hence interesting and topical. In the study of blast effects inside monumental structures, a particular attention must be paid to the procedure to be used for numerical simulations, that must account, on one hand, for the hypervelocity of the phenomenon and, on the other hand, for reflected shock waves. In fact, the internal geometry of a monument, often rather complex, can alter significantly the time history of the reflected blast pressure on the walls and some peculiar phenomena can happen, leading to an abnormal increase of the shock pressure and also to an unconventional time distribution of it. Another peculiarity of monumental structures is the type of the material. Normally composed of stones or masonry, the constitutive law of the material must be able to describe cracks produced by the blast and propagating into the body of the structure, which needs the use of a nonlinear model for the behavior of the material. In this communication, we propose first a comparative study on different methods for the evaluation of the blast pressure field inside a typical monumental structure: a vaulted hall. We compare empirical models (CONWEP and the recommendations TM5-1300 of USACE) with a completely numerical simulation, based upon the use of the JWL model. We give also new accurate analytical expressions for the Kingery and Bulmash experimental data, valid over the whole range of the scaled distance. The results of this study show that the shock waves reflected by the vault are focused leading to a large increase of the shock pressure. Such a result shows the importance of using numerical simulations for the calculation of blast pressure shock waves inside a monumental structure: recommendations using empirical formulations and relating to conventional geometries are inappropriate. We then apply this numerical approach to the study of a real structure: the Pantheon of Rome. A complete study, simulating the blast and the whole structure, is conducted and the consequences of the blast on the structure are completely simulated. Also in this case, we show that the focus of reflected waves is determinant in the structural collapse. The role played by the existing cracks in the Pantheon's dome is also analyzed.

Effect of Sclerostin Inhibition on Bone Mechanical Properties in a Murine Model of Osteogenesis Imperfecta as Revealed by Micro Finite Element Analysis

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ABSTRACT

Osteogenesis imperfecta (OI) is a heritable bone fragility disorder caused in the majority of cases by mutations in type I collagen, leading to reduced bone mass, brittleness and deformities. Limitations in current treatment strategies may be overcome by anabolic sclerostin neutralizing antibody (Scl-Ab) therapy. The *Brtl/+* mouse model of Type IV OI recapitulates the main features of the OI phenotype. The aim of this work is to determine the influence of Scl-Ab treatment on the mechanical behaviour of normal and *Brtl/+* murine bone. In previous work, femora from two wildtype (WT) and two *Brtl/+* male, 6 month old mice were treated with vehicle (saline) or Scl-Ab (BPS804, Mereo BioPharma) (n=1/genotype/treatment). Scl-Ab or vehicle was administered via intravenous injection for 5 weeks in a dose of 100 mg/kg/week. Each bone was scanned by lab micro computed tomography at 10 μm resolution and a mid-shaft region was imaged with phase-contrast synchrotron radiation-source CT (SR-CT, ESRF ID19, France) at 650 nm voxel size. In this study, micro finite element (microFE) models are developed to investigate the bone properties on two length scales. On the one hand, an organ-scale model of the entire femur is generated from the segmented microCT images. Material properties are assumed to be homogeneous and linear elastic, with Young's moduli of bone tissue in the WT and *Brtl/+* femora determined from recent nanoindentation data [1]. The models are loaded in a four-point bending setup to evaluate stiffness and estimate strength. On the other hand, a meso-scale model is created from the segmented SR-CT images of the mid-shaft region and subjected to axial compression and bending. The role of tissue inhomogeneity is investigated by assigning individual elastic properties to the bone elements based on the local SR-CT density [2] and comparing the results to the homogeneous models. Further, the effect of cortical porosity is evaluated by turning lacunar porosity on/off in the models. The results of the WT and *Brtl/+* mice are compared to evaluate the effect of the disease. The influence of the treatment is assessed by comparing the properties of the Scl-Ab-treated and the vehicle-treated animals. The findings will help to better understand the effect of Scl-Ab treatment on the mechanical properties of OI-bone and provide insight into the contributions of bone matrix heterogeneity and porosity. 1. Sinder et al. *J Bone Miner Res.* 2013, 28(1):73-80. 2. Razi et al. *Acta Biomaterialia*, 2015, 13:301-10.

Cross Migration of Surfactant-laden Viscous Droplets in a Transient Stokes Flow

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ABSTRACT

We consider the motion of a viscous drop in an arbitrary unsteady Stokes flow such that the surface of the drop is fully covered with a stagnant surfactant layer. In particular the regime of low surface Péclet number is analyzed and we account for the effect interfacial slip on the overall behavior of the flow field. The hydrodynamic problem is solved by the solenoidal decomposition method and the drag force is computed in terms of Faxen's laws, using a perturbation ansatz in powers of the surface Péclet number. The surface equation of the deformed sphere has been determined by an iterative method up to the first order approximation. Analytical expressions for the migration velocity of the drop are likewise given. Based on this analysis we can completely characterize various flow situations including a given ambient flow as uniform flow, Couette flow and Poiseuille flow. Moreover, we find out that a surfactant-induced cross-stream migration of the drop occurs towards the centre-line in both, Couette and Poiseuille flow cases. The variation of the drag force and the migration velocity is computed for different parameters such as the Péclet number and the Marangoni number. Finally, the theoretical findings are validated on with available experimental data.

Predictive Model for Porosity in Powder-bed Fusion Additive Manufacturing in the High Energy-density Regime

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ABSTRACT

Process consistency and control are bottleneck issues to wider insertion of powder-bed fusion additive manufacturing in the industrial shopfloor. Of particular interest is the porosity of the components, which remains the limiting factor to high-cycle fatigue performance. Recent experiments have shown that, with increasing energy density, a surge in porosity is seen in selectively laser melted metals. In this high-energy density regime, porosity originates from mechanisms that have to be different from the well-known incomplete melting occurring in the low energy density regime. To shed light on this interesting phenomenon, we discuss the mechanism of bubble formation in the melt pool and possible trapping during the solidification, and then we formulate a predictive model for porosity in this regime. To compare with experimental results, we perform computer modelling and simulations (which have been validated by experiments) to determine the parameters of the model. We show that the model predictions are in reasonable qualitative and quantitative agreement with the experimental measurements. Hence, the proposed model can be used as a tool to predict porosity at increasing beam energy density, and further to control and possibly reduce it, paving the way for wider adoption of powder-bed fusion additive manufacturing in modern shopfloors.

Micro/meso-scale Modeling of 3D Woven Composites with Temperature Dependent Properties of Constituents

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ABSTRACT

In this research we investigate how the overall response and local stress concentrations in the 3D woven composites are influenced by the temperature dependence of constituents. We utilize our recently developed meso-scale finite element models of the material [1-2] and study responses of individual fiber tows and the entire composite unit cells. The considered loading cases include cooling of completely cured composite from curing to room temperature and thermo-mechanical loading in the range of service temperatures. Temperature dependent effective elastic properties and overall thermal expansion coefficients are obtained from the simulations. Studies of carbon reinforced epoxies show that the temperature dependent effects are well pronounced in the overall response and can lead to significant local stress concentrations. [1] A. Drach, B. Drach, I. Tsukrov. Processing of Fiber Architecture Data for Finite Element Modeling of 3D Woven Composites, *Advances in Engineering Software*, v 72, pp. 18–27, 2014. [2] I. Tsukrov, B. Drach, A. Drach, T. Gross. Utilizing Stress-based Failure Criteria for Prediction of Curing Induced Damage in 3d Woven Composites, *Proceedings of 21st International Conference on Composite Materials – ICCM21*, Xi'an, China, 2017.

Hierarchical Validation of the WIAMan LS-Dyna FEM for Application in Underbody Blast

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ABSTRACT

A finite element model (FEM) has been developed in conjunction with the development of the Warrior Injury Assessment Manikin (WIAMan) Anthropomorphic Test Device (ATD) and will serve as a state of the art Soldier surrogate for Underbody Blast (UBB) testing. The FEM will complement the physical ATD to predict injury response and assess operational risk of ATD failure. The objective of this work is to present the validation of the WIAMan FEM in sub-system and system-level simulations. The WIAMan FEM was developed and validated using a hierarchical approach. Component models were developed and validated individually and incorporated into the full system-level model. Validation of the component models occurred in two sets of experiments, non-injurious and injurious loading conditions. The test articles for these simulations were the lower leg, pelvis, and lumbar spine. The whole body model contains ~1.4 million nodes and was simulated in three loading conditions. Two whole body conditions were simulated from the Vertically Accelerated Load Transfer System (VALTS) test series, an upright posture and a reclined-seatback posture with the legs extended. The remaining simulation was of a test series run at the University of Michigan with the legs at an acute angle under the body. Model validation was quantified using 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 whole body WIAMan FEM is approximately 13 hours for a 100 ms simulation on 100 processors. Preliminary results of the component simulations show good agreement with the experimental response. CORA scores for the components range from 0.62 to 0.83 across all input conditions. In whole body simulations, 33 signals were evaluated for each of the three whole body simulations including accelerations, rotations, forces, and moments. Preliminary results indicate a strong match to the experimental response with a CORA score of 0.76 in the nominal posture VALTS simulation. The validation results give confidence in the FEM's ability to predict the ATD response to a variety of loading conditions and encourage future use in designing safety measures for the warfighter in UBB. This study was part of the WIAMan Research sponsored by the U.S. Army Research Laboratory. The content included in this work does not necessarily reflect the position or policy of the U.S. government.

A Second-order Cone Interior-point Method for Initially Rigid Cohesive Fracture

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ABSTRACT

Initially rigid cohesive fracture is among the few techniques able to model complex and branching fracture with a sharp (nonsmeared) representation of the crack. Implicit time-stepping schemes are often favored in mechanics due to their ability to take larger time steps, but it is challenging to include an initially rigid cohesive model in an implicit scheme because the initiation of fracture corresponds to a nondifferentiability of the underlying potential. In this work, an interior-point method is proposed for implicit time stepping of initially rigid cohesive fracture. It uses techniques developed for convex second-order cone programming for the nonconvex problem at hand. The underlying cohesive model is taken from Papoulia (2017) and is based on a nondifferentiable energy function. That previous work proposed an algorithm based on successive smooth approximations to the nondifferential objective for solving the resulting optimization problem. It is argued herein that cone programming can capture the nondifferentiability without smoothing, and the resulting cone formulation is amenable to interior-point algorithms. A further benefit of the formulation is that other conic inequality constraints are straightforward to incorporate. A computational result is provided showing that certain contact constraints can be easily handled and that the method is practical.

Multiple Necking Pattern in Nonlinear Elastic Bars Subjected to Dynamic Stretching: The Role of Defects and Inertia

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ABSTRACT

In this work we explore the inception and development of multiple necks in incompressible nonlinear elastic bars subjected to dynamic stretching. The goal is to elucidate the role played by a spatial-localized defect of the strain rate field in the necking pattern that emerges in the bars at large strains. For that task, we have used two different approaches: (1) finite element simulations and (2) linear stability analyses. The finite element simulations have revealed that, while the defect of the strain rate field speeds up the development of the necking pattern in the late stages of the localization process, the characteristic (average) neck spacing is largely independent of the defect within a wide range of defect amplitudes. The numerical results have been rationalized with the linear stability analyses, which enabled to explain the average spacing characterizing the necking pattern at high strain rates. Moreover, the numerical calculations have also shown that, due to inertia effects, the core of the localization process occurs during the post-uniform deformation regime of the bar, at strains larger than the one based on the Considère criterion. This phenomenon of neck retardation is shown to have a meaningful influence on the necking pattern.

Mechanical Instability of an Origami-Inspired Cellular Structure

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ABSTRACT

In this project, we present a novel group of origami inspired cellular structures with reversible foldability and programmable instability. The mechanical instability of these structures relies on the properties of the material, hinge pattern, and hinge characteristics. The unit cell of the proposed cellular structure is a star-shaped sub-assembly with either one or two zero-energy states. Applying an external load on the unit cell, while it is initially in the first stable configuration and has zero energy, increases the level of energy up to a turning point and in some cases recovers the zero energy level corresponding to another stable configuration. Here, we investigate the instability of the structure experimentally and then explore the influence of geometrical parameters on the existence and quality of bi-stability through an analytical approach. The instability of the star-shaped unit cells can be further programmed by forming different styles of stars (three-pointed star, four-pointed star, and etc.) which alter the mechanical properties as well as the instability of the structure. The instability characteristics of the unit cells (mostly bi-stability) get transferred to a higher order structure which is made by tiling the star-shaped unit cells in three dimensions. Another fascinating feature of the star-shaped unit cell which gets extended to the cellular structure is auxeticity (i.e. negative Poisson's ratio). A careful observation indicates the reduction of the cross-sectional area of the unit cell under compressive load until it ends in a smaller cross-sectional area compared to the first zero-energy configuration.

Simulation of Flat Carbon Fibre Reinforced Laminated Composite Plates Subjected to Axial Crushing: Comparison of Two Intra-Laminar Damage Models in LS-DYNA and ABAQUS/Explicit

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ABSTRACT

Carbon Fibre Reinforced Polymer (CFRP) systems are being widely used for crashworthy structural applications in the aerospace and automobile industry. The numerical prediction of the crushing response of CFRPs is challenging due to the complex nature of the various interacting failure modes that occur at different length scales. In this work, two intra-laminar damage models with different underlying assumptions are used to predict the mass-specific energy absorption (SEA) of flat coupon specimens made from IM7/8552 CFRP under dynamic axial crushing. The sub-laminate based continuum damage model, CODAM2 [1], implemented in LS-DYNA as the material model MAT_219 is compared to a ply-based damage model based on the Ladevèze theory [2] and implemented as a user subroutine (VUMAT) in ABAQUS/Explicit. The sensitivity of different CFRP layups on the SEA is numerically studied to investigate the capability of the two intra-laminar damage models to predict those layup variations. Results are compared with experimental data provided by the University of Utah [3]. This study demonstrates the capabilities, effects of various parameters and material model specific options and limitations of both damage models, thus contributing to further understanding and improvement of the structural analysis of composites under dynamic loading conditions such as crash or high velocity impact events. [1] A Forghani, N Zobeiry, A Poursartip and R Vaziri (2013). A structural modelling framework for prediction of damage development and failure of composite laminates, *Journal of Composite Materials*, 47(20-21), 2553–2573. [2] P Ladeveze, P and E LeDantec (1992). Damage modelling of the elementary ply for laminated composites. *Composites science and technology*, 43(3), 257-267. [3] M Perl, D Adams. Phase III Flat Coupon Crush Test Results, CMH-17 Crashworthiness WG Meeting, September 5, 2017.

A Multi-Physics Approach to Predicting Separation Forces in Constrained-Surface Stereolithography

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ABSTRACT

Constrained-Surface Stereolithography (SL) is an additive manufacturing technology that prints three-dimensional objects by selectively exposing a liquid pool of photosensitive resin to UV radiation. A typical Constrained-surface SL apparatus consists of (a) Build platform (b) Resin vat and (c) Digital Imaging unit. The apparatus is used to print the object in a bottom-up approach, wherein the first layer is bonded onto the build platform and subsequently each new layer is printed in the gap between the bottom surface of the previously printed layer and the top surface of the resin vat. The build platform is maneuvered upwards upon the completion of each layer, to replenish the liquid volume in the gap. This separation is resisted by viscous adhesion due to the presence of the resin between the bottom surface of the part and the top surface of the vat. This adhesion poses a major hurdle to printing parts with a characteristic axial length of order of 10 mm. This adhesion can be attributed to a pressure gradient associated with the flow of the viscous resin into the gap. One of the most efficient strategies to reduce this adhesion is to coat the bottom surface of the vat with a thin film of an optically transparent and inert material (e.g. PDMS, Teflon, PTFE). The reduction in the adhesion is achieved via an elastohydrodynamics phenomenon involving a coupling of liquid flow and elastic deformations of the film in the gap. This work develops a theoretical framework to establish the dependence of the separation force on the mechanical properties of the liquid resin and the film coating. The flow of the resin into the thin gap between the part and the film is modeled using lubrication theory [2] while the elastic deformations of the thin film coating are modeled using perturbation theory [1]. A Finite Element (FE) model is developed on the basis of the resulting system of partial differential equations using a mixed Finite Element (FE) framework. Finally, the FE model is employed to predict the separation force on a printed part separating from a film for a constant build-platform speed. Bibliography [1] Argatov, Ivan and Gennady Mishuris. Contact Mechanics of Articular Cartilage Layers Asymptotic Model. Switzerland: Springer International Publishing, 2015. [2] Szeri, Andras Z. Fluid Film Lubrication: Theory and Design. Cambridge University Press, 2005.

Stabilization of XFEM Formulations by Tikhonov Regularization and Modified Barzilai-Borwein Iteration

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ABSTRACT

In some cases the eXtended Finite Element Method may show ill-conditioning of the global system of equations at solution due to near linear dependency between element shape functions and enrichment functions. For example, this is easily observed when a discontinuity crosses nearby the element nodes and the Heaviside function enrichment is present. In [1] it has been shown that ill-conditioning has, as limiting case, the indeterminacy of the global system of equations. This originated the idea of improving system conditioning by biasing to zero a proper subset of the enrichment variables by a weak penalty term. This technique can be seen as a particular case of Tikhonov regularization [2], that is one of the most commonly used methods of regularization of ill-posed problems in statistics and analysis of inverse problems. The attractive properties of this stabilization technique is that it has no impact on the XFEM formulation, can be used for any set of enrichment functions and is of straightforward implementation. The introduction of the penalty term introduces a bias in the solution, whose entity can be considered acceptable in most applications. However, it is desirable that the solution is not affected by the stabilization procedure. To this end various alternatives has been explored: fixed point iteration with a correction term on the final solution system and several forms of the augmented lagrangian method. Nonetheless, all these alternatives were found not efficient from a computational point of view. Recently, an efficient way of eliminating the stabilization bias from the solution has been found by developing a new iteration formula that sets its roots on the method proposed by Barzilai and Borwein [3], who suggested formulas for the stepsize determination in steepest descent methods. The derived new iteration formula shows very good performance and leads to convergence in a few iterations. In the present contribution the derivation of the new iteration formula is shown and examples of its application to the stabilization of XFEM problems are given. [1] G. Ventura, C. Tesei. Stabilized X_FEM for Heaviside and nonlinear enrichments. In *Advances in Discretization Methods*, pages 209–228, Springer, 2016. [2] A.N. Tikhonov, A.V. Goncharky, V.V. Stepanov, and A.G. Yagola. *Numerical methods for the solution of ill-posed problems*, volume 328. Springer Science & Business Media, 2013. [3] J. Barzilai, J.M. Borwein. Two-Point Step Size Gradient Methods, *IMA Journal of Numerical Analysis*, Volume 8, Issue 1, 1 January 1988, Pages 141–148.

Biomechanics of the Fetal Kicking Linked to Risk Factors for Developmental Dysplasia of the Hip

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ABSTRACT

INTRODUCTION: Developmental dysplasia of the hip (DDH) is a common congenital joint shape malformation, associated with an increased risk of osteoarthritis in later life [1]. Risk factors for DDH are associated with restricted fetal movement, such as fetal breech position and low amniotic fluid volume (oligohydramnios) [2]. In addition, first-borns are significantly more likely than consecutive births to develop DDH [3]. However, counter-intuitively, DDH is not more common in twins despite significantly less space available for each fetus [4]. By quantifying the mechanical stimulation of the fetal skeleton for a range of uterine conditions which increase the risk of DDH, we test the hypothesis that a biomechanical link exists between fetal kicking and the occurrence of DDH. **METHODS:** Fetal biomechanics were modeled for cine-MRI scans of normal, cephalic fetuses, and fetuses in breech, oligohydramnios or twin pregnancies (n=3-7 per group) [5]. Muscle forces were applied to finite element models of two different geometries of fetal bones generated from post-mortem MRI. **RESULTS:** Maximum fetal kick force and resulting stress stimulation were significantly lower in breech and oligohydramnios scans, while there was no significant difference for twin kicks, compared to normal singletons (Figure 1B, C). The reaction force was significantly lower in firstborn fetal kicks, with downward trends in stress stimulation. **DISCUSSION:** This study reveals significant decreases in biomechanical stimulation of the hip joint in cases of breech and oligohydramnios, known risk factors for DDH. Furthermore, there were no significant differences between singleton and twin pregnancies, despite the more restrictive mechanical environment, possibly explaining the normal incidence of DDH in twins [4]. This work sheds new light on a potential biomechanical link between fetal movements and the development of DDH. **REFERENCES:** 1. Sandell, Nat Rev Rheumatol, 8:2, 2012 2. Hinderarker et al, Acta Orthopaedica, 65:3, 1994 3. de Hunt et al, Eur J Obst Gyn Reprod Biol, 165:1, 2012 4. De Pellegrin et al, J Pediatr Ortho, 30:8, 2010 5. Verbruggen et al, Biomech Model Mechanobiol, 2016 **ACKNOWLEDGEMENTS:** Arthritis Research UK (20683) Wellcome Trust and EPSRC iFind project (102431), ERC dHCP project (FP2007-2013 319456), NIHR-CS-012-002, NIHR GOSH.

Skeleton-stabilized Immersed Isogeometric Analysis for Incompressible Flow Problems

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ABSTRACT

Isogeometric Analysis (IGA) of incompressible flow problems has been an active topic of research over the last decade. In particular, IGA of mixed formulations for incompressible flow problems based on inf-sup stable velocity-pressure pairs has been demonstrated to be very suitable, which has led to the development of a range of isogeometric element families. In recent years, it has been shown that direct application of these element families in an immersed (Isogeometric Finite Cell) setting leads to local oscillations in the pressure field near cut boundaries. In this contribution we present an alternative stabilization technique that avoids the stability problem observed for inf-sup stable velocity-pressure pairs in the Isogeometric Finite Cell method. The pivotal idea of the considered technique is to control the jump of high-order derivatives of the pressure field over the skeleton structure of the mesh. This skeleton-based stabilization technique allows utilizing identical discrete spaces for the velocity and pressure fields. To enable application of the skeleton-based stabilization technique in the Isogeometric Finite Cell setting, the system is complemented with a stabilization term for the velocity space similar to that of the pressure space. In contrast to the pressure stabilization, the velocity stabilization – which is referred to in the literature as Ghost-penalty stabilization – is only applied at the faces of the background mesh skeleton structure that are located near the cut boundaries. Since the proposed skeleton-based stabilization technique is applicable in the conforming setting, we have studied its performance for a range of Stokes flow and moderate Reynolds number Navier-Stokes flow benchmark problems on two and three-dimensional conforming meshes, including the case of a multi-patch NURBS-based Isogeometric Analysis. We have observed the skeleton-based stabilization method to yield solutions that are free of pressure oscillations and velocity locking effects, and to yield optimal rates of convergence under mesh refinement. The observations for the conforming isogeometric setting extend to the immersed setting, where we have considered a range of two and three-dimensional problems for incompressible flows. To demonstrate the versatility of the proposed simulation strategy we have considered the Isogeometric Finite Cell analysis of Stokes flow through a porous medium, where the geometry is extracted directly from three-dimensional scan data.

Theory and Simulation of Fast - Travelling Dislocations: An Atomistic Perspective

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ABSTRACT

Our understanding of dislocation mobility - quantifying the relationship between the force on a dislocation and its resulting velocity - is largely based on experiment. However, the validity of mobility laws extracted from this work breaks down for fast travelling dislocations moving with speeds comparable to the speed of sound in the medium. Debate on the topic of dislocation mobility in the pure glide regime has been ongoing for over half a century. At the heart of the discussion lies the problem that in this regime, the usual approximations by which elasticity theory is linearised are violated and the quasi-static approximation no longer holds. In the last 20 years, large-scale non-equilibrium molecular dynamics simulations have been used to produce qualitative mobility laws for fast travelling dislocations. Despite the breadth of physical phenomena that are captured in these simulations, they have failed to provide the community with a general understanding of dislocation mobility in this regime. We will show how lattice-dynamics models and simulations of uniformly moving dislocations may provide an accurate description of the dislocation - phonon interactions in metals. These interactions are widely believed to play a crucial part in physical descriptions of dislocation mobility. Quantitative comparisons between the lattice dynamics model and equivalent molecular dynamics simulations will be made. Furthermore, the effect of the dislocation core width on its mobility will be presented. Finally, the consequences of these results for a more general theory on dislocation mobility in the pure glide regime will be discussed. References W.G. Johnston, J.J. Gilman, J. Appl. Phys., 30 129 (1959) Z. Jin, H. Gao, P. Gumbsch, Phys. Rev. B, 77 094303 (2008) B. Gurrutxaga-Lerma, D.S. Balint, D. Dini, D.E. Eakins, A.P. Sutton, Proc. R. Soc. A, 469 2156 (2013)

Stabilised Finite Element Methods for Variational Inequalities

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ABSTRACT

We survey our recent and ongoing work [1,2,3] on finite element methods for contact problems. In our approach, we first write the problem in mixed form where the contact pressure acts as a Lagrange multiplier. To avoid the problems related with a mixed finite element discretisation, we use a stabilised formulation, in which appropriately weighted residual terms are added to the discrete variational forms. We show that the discrete formulation is uniformly stable and that it leads to an optimal a priori error estimate. Using the stability of the continuous problem, we establish a posteriori estimates whose optimality is ensured by local lower bounds. In the implementation of the methods, the discrete Lagrange multiplier is locally eliminated, thus giving rise to a Nitsche-type method. We present a series of numerical results which support the optimality of our a posteriori estimates. [1] T. Gustafsson, R. Stenberg, J. Videman. Mixed and stabilized finite element methods for the obstacle problem. *SIAM Journal of Numerical Analysis* 55 (2017). 2718–2744 [2] T. Gustafsson, R. Stenberg, J. Videman. Stabilized methods for the plate obstacle problem. <https://arxiv.org/abs/1707.08396> [3] T. Gustafsson, R. Stenberg, J. Videman. Nitsche's method for boundary constraints (in preparation).

From Polymer Physics to Rubber Elasticity

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ABSTRACT

In this talk, I will present recent results on the ab-initio modelling of rubber-like materials. The starting point is a random network of interacting polymer chains, the free energies of which are explicit functions of the temperature, their numbers of monomers and their elongations. In a discrete-to-continuum homogenization regime, this model gives rise to continuum nonlinear elasticity. The associated energy density is characterized by an asymptotic (nonlinear) cell-problem on the discrete network. We shall describe the generation of the network, the numerical solution method, and present numerical results that compare favourably to both mechanical experiments (at the macroscopic level) and physical experiments (at the level of the network, recovering the so-called butterfly effect). This is based on joint works with L. Giovangigli and A. Gloria (Sorbonne Université), F. Lequeux (ESPCI), and P. Le Tallec (Ecole polytechnique)

On Hellinger-Reissner type Mixed Finite Elements for Hyperelasticity

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ABSTRACT

The Mixed Finite Element Method is an excellent tool for the computation of boundary value problems that involve some kind of limiting behavior. In the framework of elasticity one of the most common applications is the case of incompressibility. It is well known, that classical displacement based finite element schemes suffer from so-called locking-phenomena in these situations, see [1], whereas mixed methods perform significantly better in many cases. In this framework the formulation proposed by Pian and Sumihara [2], which is based on the Hellinger-Reissner principle, is still one of most efficient formulations available. Unfortunately, due to the use of a complementary energy, the formulation is only available in the linear elastic case and very special and limited cases of nonlinear elasticity [3]. In this work we will propose some basic ideas on the extension of the Pian-Sumihara element into a general hyperelastic framework. It will be shown that, depending on the choice of your interpolating stress-quantity, hourglass modes may occur and a stabilization is necessary. [1] I. Babuska, M. Suri, Locking Effects in the Finite Element Approximation, Numer. Math., 62:439-463, 1992 [2] T.H.H. Pian, K. Sumihara. Rational Approach for assumed stress finite elements. International Journal for Numerical Methods in Engineering 20:1685-1695, 1984 [3] P. Wriggers. Mixed Finite-Element-Methods. In: Mixed Finite Element Technologies, CISM Courses and Lectures, vol 509. Edited by P. Wriggers and C. Carstensen, 2009

Multi-Scale Constitutive Modelling of Multiphase Alloys

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ABSTRACT

Multiphase alloys, such as TRIP (transformation induced plasticity) and dual-phase steels, enjoy considerable technological importance, due to their favourable mechanical properties such as a combination of high yield strength and elongation at failure. However, complex phenomena, such as plastic slip and martensitic phase transformations, pose a number of computational challenges. A variety of phenomenological and micromechanical constitutive models have been proposed in the literature, accounting for the major features of their macroscopic behaviour. However, a large number of material parameters is usually required, limiting their predictiveness and generalisability. In this context, multi-scale models are a natural fit due to their ability to both capture the fine-scale crystalline features and connect them to the macroscopic scale. The overall material behaviour can thus be directly obtained from modelling the multiple constituent phases – slip in FCC or BCC lattices, for the ferrite, martensite and stable austenite phases, and FCC-to-BCC phase transformations, for the meta-stable austenite crystallites. Here, a fully implicit rate-dependent formulation [1], using the volume-preserving exponential map [2] and strategies such as sub-stepping is employed. Thus, the issues of rate-independent formulations, such as non-smooth yield functions, active system set search and non-unique solutions are circumvented. Additionally, the effect of mechanically-induced martensitic transformations is introduced using a recently proposed generalisation of Patel and Cohen's [3] energy-based criterion. The resulting model also includes coupling effects with the evolution of austenite slip activity, bearing many similarities with the aforementioned crystal plasticity models. Thus, analogous computational difficulties arise and are tackled similarly. In order to study the macroscopic behaviour of multi-phase crystalline materials and its intrinsic connection to their complex microstructure, a large-strain fully implicit, RVE-based multi-scale finite element code is used. Both RVE homogenisation and fully coupled (FE2) analyses are performed to study the influence of microstructural parameters on the resulting behaviour for materials of interest, for which experimental data is available, such as metastable austenitic stainless steels and TRIP steels. References: [1] R. J. Asaro and A. Needleman. "Overview No. 42: Texture Development and Strain Hardening in Rate Dependent Polycrystals". In: *Acta Metallurgica* 33.6 (1985). [2] C. Miehe. "Exponential Map Algorithm for Stress Updates in Anisotropic Multiplicative Elastoplasticity for Single Crystals". In: *International Journal for Numerical Methods in Engineering* 39.19 (1996). [3] J. R. Patel and M. Cohen. "Criterion for the Action of Applied Stress in the Martensitic Transformation". In: *Acta Metallurgica* 1.5 (1953).

Solution for Strain Softening Problem in FEM and SPH

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ABSTRACT

The main aim of this work was addressing localisation problem observed in the analysis of strain softening materials using finite element methods (FEM) and the smooth particle hydrodynamic (SPH) methods, combined with local continuum damage mechanics (CDM) approach. More specifically, the objective was to reduce and possibly remove mesh dependency of the numerical results and balance the effects of heterogeneous microstructure on local continua while keeping the boundary value problem of softening (damaged) continua well-posed. Strain softening is typically observed in damaged quasi brittle materials such as fibre reinforced composites and application of the CDM approach with the classic FEM features a number of anomalies, including mathematical (change of the type of partial differential equations leading to ill-posed boundary value problem), numerical (pronounced mesh dependency) and physical (infinitely small softening zone with the zero dissipated energy). Consequently, alternative definition of damage effects, called equivalent damage force (EDF) was proposed here, where the damage effects were solely contributing to the right-hand side of the momentum balance equations, whilst keeping the left hand side of the equation and also the type of partial differential equations unchanged, relative to the linear elastic response. The FEM and the SPH combined with a local continuum damage model (CDM) were used for analysis of a dynamic stress wave propagation problem, which was analytically solved in [1]. The analytical solution was compared to the numerical results, obtained by using a stable, Total-Lagrange form of SPH [2,3], and two material models implemented in the FEM based on: 1) classic CDM; and 2) equivalent damage force. The numerical results demonstrate that the size of the damaged zone is controlled by element size in classic FEM and the smoothing length in the SPH, which suggests that the SPH method is inherently non-local method and that the smoothing length should be linked to the material characteristic length scale in solid mechanics simulations. 1. Z.P. Bazant and T.B. Belytschko, Wave propagation in a Strain- Softening Bar: Exact Solution, *Journal of Engineering Mechanics*, 111, 381-389, 1985. 2. R. Vignjevic, N. Djordjevic, S. Gemkow, T. DeVuyt, J. Campbell, j., 2014. SPH as a nonlocal regularisation method: Solution for instabilities due to strain-softening. *Computer Methods in Applied Mechanics and Engineering*, 277, pp. 281-304. 3. R. Vignjevic, J. Campbell, J. Jaric, S. Powel, Derivation of SPH Equations in a moving referential coordinate system, *Computer Methods in Applied Mechanics and Engineering*, 198, 2403–2411, 2009.

A Three-dimensional, Mechanochemical Model of the Cellular Cortex

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ABSTRACT

The cellular cortex is a thin layer underneath the plasma membrane of animal cells. It is composed by an intertwined network of actin fibers attached by crosslinkers and myosin motors that exert contractile forces among the fibers. The cortex plays a central role in global cellular mechanics, cell shape control, morphogenesis and cytokinesis. Its misregulation is involved in several diseases. However, the cortex mechanics remains not well understood. Here we developed a continuous mathematical model to study macromechanical responses of the cellular cortex under internal stimuli and external forces. In our framework, the cellular cortex is modeled as a viscoelastic fluid that generates active stresses. Furthermore, due to the small thickness of the actomyosin network compared to the dimensions of the cell we model the cortex as a surface. Using this approach, we investigate the behavior of cells subjected to forces at different time scales as the cellular cortex responds as an elastic network under short time-scale forces, while it behaves as a viscous fluid at longer time-scales. We also study the tightly coupled dynamics of the cortex layer and the cellular plasma and how they influence cell division and migration.

Numerical Simulation of Rivulets Formation Based on a Shallow Water Type Model

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ABSTRACT

This work deals with the numerical simulation of the motion of a thin partially wetting liquid film flowing on a solid substrate. One of our objectives is to be able to predict the formation of rivulets in the case of a water film sheared by an air flow. This type of situation is encountered, for example, in the case of thermal de-icing systems for aircraft wing. The liquid film which is formed in this case is generally unstable. Rivulets are formed which radically modify the exchange area between the film, the heated wing and the air flow, and therefore play a decisive role on the efficiency of the de-icing system. Classically, the dynamic of thin liquid film is modelled by the lubrication equation (see for example [1]). This equation involves fourth order derivatives to take into account the effects of capillary forces. This may lead to numerical issues, especially in our case where we want to use an unstructured mesh finite volume solver which is well suited for industrial applications. To avoid these difficulties, the lubrication equation has been replaced in the present work by a shallow water type model, written in conservative form and involving only second order derivatives thanks to the introduction of an additional transport equation for the gradient of the film thickness (as proposed in [2]). A non-singular disjoining pressure model has been used to account for the capillary forces in the vicinity of the film contact line [3]. In addition, an implicit cell-centred unstructured finite volume scheme has been developed and implemented for the discretization of the problem. Based on this approach, many 2D and 3D simulations have been performed to assess its capability to accurately reproduce both linear stability theoretical results and experimental results for partially wetting film configurations and rivulets formation. During the conference, the model, the numerical method and the simulation results will be presented and discussed. [1] JA Diez, L Kondic. On the breakup of fluid films of finite and infinite extent. *Physics of Fluids* 19 (7), 2007. [2] P. Noble, J.P. Vila, Stability Theory for Difference Approximations of Euler-Korteweg Equations and Application to Thin Film Flow, *SIAM J. Numer. Anal.* 52(6), 2014 [3] J. Lallement, Ph. Villedieu, P. Trontin and C. Laurent, A shallow water type model to describe the dynamic of thin partially wetting films, 23ème Congrès Français de Mécanique, Lille, 2017

Computational Design Optimisation for Local Control over Mechanical Properties in Heterogeneous Scaffolds

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ABSTRACT

Introduction There is a compelling argument in favour of designing bone tissue engineering (BTE) scaffolds able to drive optimised bone formation by stimulating the mechanotransduction processes of the osteogenic cells in a controlled manner. However, in current BTE techniques, prediction, control and characterisation of the local mechanical environment created within the scaffold are insufficient. The importance of scaffold design parameters such as stiffness, pore size and pore shape for tissue growth has been established [1] but most scaffold designs still neglect the considerable heterogeneity observed in native bone architecture. The authors have implemented a digital tool for automated computer design of heterogeneous scaffolds with local mechanical properties and porosity optimized for user-specified objectives. The main goals of this study were to characterise the fidelity of the 3D printed constructs to the designs, validate the predictive computational scaffold models, and assess the performances of the optimisation procedures via in-silico and in-vitro testing. Methods and results The design tool was implemented in C# as a plugin to the 3D modelling software Rhinoceros 3D and its algorithmic modelling platform Grasshopper. This plugin supports automatic cellular topology generation and optimisation of thicknesses of the individual cell struts to meet both local strain and porosity targets under a specified load case, building on a heuristic strain-based optimisation algorithm derived by the authors [2]. The design framework was assessed in-silico and in-vitro for compression and three-point bending scenarios by comparing the resulting optimized designs with controls, defined as homogeneous scaffolds with same outer shape and same mass as the optimized designs. CAD models of all designs were manufactured in a photocurable acrylic resin using direct light processing and mechanically tested using the simulated scenarios. Manufacture artefacts such as left-in non-cured material were incorporated into the Finite Element (FE) models. A good fidelity of the prints to the designs was observed for scaffolds with resolution $\approx 0.1\text{mm}$. The computational models accurately predicted sample stiffness ($\pm 5\%$), material failure ($\pm 5\%$) and structural failure ($\pm 10\%$). The optimised samples showed up to 40% higher material failure load than the controls. Local mechanical characterisation will be conducted using microcomputed tomography. First public release of the design software is planned for June 2018 to support researchers and clinicians unfamiliar with programming and optimisation techniques in designing reliable BTE scaffolds. References [1] Hollister SJ, Nature Materials, 4, 2005. [2] Phillips ATM, et al., International Biomechanics, 2, 2015.

Adjoint Based Optimization of a Supersonic Separator

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ABSTRACT

An emerging technology for separating gaseous mixtures, these devices expand the fluid to supersonic speeds through a convergent-divergent nozzle, so as to condense components that have higher liquefaction temperatures. The introduction of swirl causes the heavier liquid phase to be centrifuged toward the wall, where it is collected. Widely recognized for their compactness and for the absence of moving parts, the supersonic separators are deemed an attractive alternative for removing contaminants from natural gas, wherever the available space is severely limited, such as in oil rigs. Yet they still pose some significant technical hurdles. Shock waves can seriously hamper the device efficiency, as a sudden rise in temperature may stop the liquefaction process or even cause the condensate to re-evaporate. Thermodynamics modeling of fluid behavior and state equations must account for the saturation region and phase change. In addition, the vanes that cause the flow to swirl must be carefully designed, so as not to interfere with the supersonic expansion, itself. In view of these challenges, we attempt an adjoint based computation of sensitivities and optimization of the device. To that end, we make use of the SU2, an open-source suite of tools for performing CFD simulations and optimization, which includes non-ideal gas models that are crucial for the problem. References: M. Pini, S. Vitale, P. Colonna, G. Gori, A. Guardone, T. Economon, J.J. Alonso and F. Palacios "SU2: the Open-Source Software for Non-ideal Compressible Flows"; 1st International Seminar on Non-Ideal Compressible-Fluid Dynamics for Propulsion & Power IOP Publishing IOP Conf. Series: Journal of Physics: Conf. Series 821 (2017) 012013 doi:10.1088/1742-6596/821/1/012013, 2017. S. Vitale, M. Pini, P. Colona, G. Gori, A. A. Guardone, T. D. Economon, F. Palcios and J.J. Alonso "Extension of the SU2 Open Source CFD code to the simulation of turbulent flows of fluids modelled with complex thermo-physical laws"; AIAA Paper, 2760, 2015.

Computational Unsaturated Poromechanics Enhanced by Deep Learning

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ABSTRACT

Many engineering applications and geological processes involve unsaturated porous media across multiple length scales (e.g. rock joints, grain boundaries, deformation bands, and faults). Understanding the multiscale path-dependent hydro-mechanical responses of these interfaces across length scales is of ultimate importance for applications such as CO₂ sequestration and hydraulic fracture. Nevertheless, unlike the saturated counterpart, the path-dependent behaviors of the unsaturated porous media may originate from both the irreversible damage and plasticity of the solid skeleton, the hysteresis of the water retention behaviors and the resultant path-dependent hydraulic responses. For convenience, numerical models often neglect the hysteresis effect of the retention curves. This simplification often leads to unrealistic predictions. In this work, we introduce a hybrid hand-crafted/machine-learning model in which we combine a class of recurrent neural network model (based on long-short-term-memory neuron) that replicates the path-dependent water retention behaviors and classical constitutive critical state plasticity model to replicate the hydro-mechanical responses of unsaturated porous media. This approach allows one to bypass the need of deriving complex phenomenological law for the portion of the constitutive model that lacks clean physical underpinnings while retaining the part of the model that can be justified with sufficient physical arguments (e.g. critical state plasticity). A set of numerical experiments are used to demonstrate the robustness of the proposed model.

Designing Conforming Metamaterials in Irregular Domains Using Topology Optimization and Computational Conformal Geometry

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ABSTRACT

Metamaterials are artificial materials which possess superior effective properties to conventional materials. The properties of these designs are based on the repetition in 2 or 3 dimensions of a unit cell, which acts as a building unit for a metamaterial structure. Over the last decades, topology optimization methods have joined traditional conceptual designing techniques, and have been widely employed in designing metamaterial unit cells. To use these materials in actual applications, it is common practice that the unit cell is placed in specific domains acting as an infill. Apart from special cases where the unit cell is used in a 2D or 3D rectangular domain, other applications may require multiple unit cell designs to be placed in an arbitrary external geometry. In these applications, the designer faces two challenges: connectivity problems between multiple metamaterial designs, and mapping a set of rectangular unit cells on an irregular domain. A simple approach for the former is adding a boundary box surrounding groups of metamaterials, or even every metamaterial design, which leads to limiting the designing freedom of potential designs by locking material at the boundaries during the optimization. For the latter, a current approach consists of a simple repetition of the unit cell to a perfect rectangular domain, placement of the resulted structure to the actual domain, and finally trimming the structure located outside the domain. However, this method has several drawbacks, including the potential existence of overhanging structures or abandoned material islands and the significant change of the effective properties of the partial unit cells near the boundaries of the domain. In this work, we employ the conformal mapping theory to map multiple metamaterial microstructures on irregular domains, considering geometric constraints during the optimization. Using conformal mapping leverages the problem currently faced. Conformal mapping, which is an angle-preserving Riemann mapping that preserves the local shape, can efficiently transform a rectangular unit cell to an irregular quadrilateral domain. Any arbitrary domain can be discretized into a quad domain, where the main part can consist of rectangular quads leaving irregular quads mainly near the boundaries. The proposed method successfully maps more than one different unit cell designs, conformed to the external boundaries. We investigate the preservation of the effective properties compared to the traditional trimming technique and the effective properties of the original unit cell.

Evaluation of Implicit-Explicit, Additive Runge-Kutta Method Efficiency in Simulating Global Non-Hydrostatic Atmospheric Dynamics for Earth System Modeling

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ABSTRACT

A standard global atmospheric model is comprised of the Euler equations coupled with an equation of state that is a modified ideal gas law. This system of equations includes acoustic waves that must be simulated in a stable manner despite that their effect on atmospheric dynamics is usually negligible. Furthermore, this system is solved on computational grids that are typically more refined in the vertical direction to account for the shorter vertical length scales present in atmospheric physics. Thus, the discretized system contains stiff elements both from the presence of acoustic waves in the model equations and from the domain discretization. For this discretized system, the use of explicit time integration methods imposes too strict of a timestep restriction for the timescales of earth system modeling. Fully implicit methods may circumvent this timestep restriction, but a global simulation results in a massive nonlinear system that is too computationally expensive to solve at every timestep. Thus, the class of Implicit-Explicit (IMEX), Additive Runge-Kutta (ARK) methods is investigated. In particular, the ability of these methods to accurately simulate atmospheric dynamics at large timesteps is evaluated. Various approaches to splitting the model equations into stiff components, which are treated implicitly, and non-stiff components, which are treated explicitly, are explored. The Suite of Nonlinear and Differential/Algebraic Equation Solvers (SUNDIALS) package is used to quickly incorporate IMEX, ARK methods into the High-Order Methods Modeling Environment (HOMME) dynamical core within the Energy Exascale Earth System Model (E3SM). Both existing methods, as well as ones that were recently developed for this specific discretized system, are considered. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC.

Computing Solution-compensation Spaces for Robust Non-linear Systems Design

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ABSTRACT

Tolerance to parameter variation due to lack-of-knowledge or epistemic uncertainty in mechanical non-linear systems design can be improved by computing so-called Solution Spaces. They are defined as sets of good designs reaching all design goals. Box-shaped Solution Spaces are subsets of the complete Solution Space. They can be expressed as the Cartesian product of permissible intervals for the design variables. These intervals are decoupled while also allowing for unintended variations of component properties. Since the size of the permissible intervals for crucial design variables is often not large enough to account for all uncertainties and to ensure feasibility, solution-compensation spaces were introduced. Solution-compensation spaces enable increased permissible intervals. In order to compute solution-compensation spaces the design variables are divided into two groups, early- and late-decision variables. Early-decision variables are associated with permissible intervals on which they may assume any value. Late-decision variables are associated with intervals where they can be adjusted to any specific value. Solution-compensation spaces are regions of early- and late-decision variables. For all values of early-decision variables values exist for late-decision variables such that all design requirements are satisfied. Existing algorithms optimize the size of box-shaped solution-compensation spaces for linear systems. A new approach to compute solution-compensation spaces for non-linear, high-dimensional design problems is introduced. It combines an existing heuristic with the solution-space algorithm introduced in [Zimmermann & Hoessle 2013]. Starting from a good design point, a candidate box is iteratively evaluated and modified. The evaluation is performed by Monte Carlo sampling for the early-decision variables in combination with heuristic optimization for the late-decision variables. This approach is applied to a non-linear design problem within the field of vehicle dynamics.

Sharp Algebraic and Total A Posteriori Error Bounds for h and p Finite Elements via a Multilevel Approach

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ABSTRACT

We derive guaranteed, fully computable, constant-free, and sharp upper and lower a posteriori estimates on the algebraic, total, and discretization errors of finite element approximations of the Poisson equation obtained by an arbitrary iterative solver. The estimators are computed locally over patches of mesh elements around vertices and are based on suitable liftings of the total and algebraic residuals. The key ingredient is the decomposition of the algebraic error over a hierarchy of meshes, with a global solve on the coarsest mesh. Distinguishing the algebraic and discretization error components allows us to formulate safe stopping criteria ensuring that the algebraic error does not dominate the total error. We also prove equivalence of our total estimate with the total error, up to a generic polynomial-degree-independent constant. Numerical experiments illustrate sharp control of all error components and accurate prediction of their spatial distribution in several test problems. These include smooth and singular solutions, higher-order conforming finite elements, and different multigrid methods as well as the preconditioned conjugate gradient method as the iterative solver.

Modeling the Cellular Cortex as a Surface Active Gel

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ABSTRACT

We consider an active gel model for the cellular cortex, derive step by step the corresponding equations as a thin film limit, discuss numerical approaches for the proposed vector- and tensor-valued surface partial differential equations, show examples demonstrating the delicate interplay between topology, geometry and defect dynamics and relate the results to experiment for axis formation in *C. elegans* embryos.

Fracture as Material Sink

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ABSTRACT

Cracks are created by massive breakage of molecular or atomic bonds. The latter, in its turn, leads to the highly localized loss of material, which is the reason why even closed cracks are visible by a naked eye. Thus, fracture can be interpreted as the local material sink. Mass conservation is violated locally in the area of material failure. We consider a theoretical formulation of the coupled mass and momenta balance equations for a description of fracture [1]. Our focus is on brittle fracture and we propose a finite strain hyperelastic thermodynamic framework for the coupled mass-flow-elastic boundary value problem. The attractiveness of the proposed framework as compared to the traditional continuum damage theories is that no internal parameters (like damage variables, phase fields etc.) are used while the regularization of the failure localization is provided by the physically sound law of mass balance. References [1] Volokh KY (2017) Fracture as a material sink. Materials Theory 1:3

Smarter Production Technology: an Example of a Smart Bending Machine

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ABSTRACT

The so-called third industrial revolution (or Industry 3.0) brought about computer-aided manufacturing and automation, which allowed achieving unprecedented precision and reliability of production processes. However, Industry 3.0 machines come as they are, and do not change throughout their lifetime. The current trend of automation and data exchange in manufacturing industry or Industry 4.0 strives to change this position towards cyber-physical machines that communicate within the production chain and learn from shared knowledge. In this work, we apply the methodology of Industry 4.0, namely Internet of things and machine learning, to the state-of-the-art sheet metal bending technology. Two typical problems of sheet metal forming are considered: an incorrect labeling of sheet metal plates or material identification, and an inaccurate prediction of the technological parameters or process characteristics prediction. These two problems are considered as building blocks of a smart bending machine and are solved for the test case of the air bending operation based on an available extensive experimental database. Material identification is implemented as a classification problem, where five classes of materials are considered (aluminum, structural steel, stainless steel and high-strength steel). A number of classification methods have been tested and the best of them allowed predicting the material class with 95% of accuracy based only on limited information (namely the springback value, and tooling and plate dimensions). Further, based on the identified material classes, a prediction model based on regression prediction has been trained. As for the material classification, a number of methods have been tested and compared as between different trained regression models, and also with the existing analytical model. The results revealed that even 200 tests are enough to train the regression model of the air bending process to achieve a springback prediction error below 5%, while the initial prediction error was above 12%. Given the communication between smart bending machines for the data acquisition, the material detection and bending parameters can be significantly improved very rapidly, since only a limited number of training data are necessary.

Multiscale Modeling of Ground Motions from Underground Explosions

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ABSTRACT

This work describes a methodology used for large scale modeling of wave generation and propagation from underground chemical explosions conducted at the Nevada National Security Site (NNSS) fractured granitic rock. We show that the discrete natures of rock masses as well as the spatial variability of the fabric of rock properties are very important to understand ground motions induced by underground explosions. Parallel codes are used to model physical processes at various scales. In the close vicinity of the source on the scale of 1-10 m, we apply a massively parallel Eulerian hydrocode, GEODYN with adaptive mesh refinement to model the shock wave generation around the source. This code supports large material deformations which may take place near the cavity created around the source. Eulerian solution is later remapped onto a Lagrangian parallel hydrocode, GEODYN-L, which explicitly accounts for discontinuities in the rock mass. The presence of joints and geologic layers may lead to elastic-plastic anisotropy of the rock mass. Explicit representation of these discontinuities is computationally expensive since it requires to use mesh resolution comparable to the joint density which is of the order of 1 m. We apply this method in the range where the rock mass response is not elastic (< 100 m). Beyond this range the rock mass can be considered elastic and can be represented by an anisotropic continuum model. Effective anisotropic stiffness for the rock mass is calculated by upscaling procedure where contribution of both the rock and the joints are used. This approach allows us to propagate seismic waves applying linear elastic anisotropic model to 1-10 km range. Thus, the ground motion generated in the near-field is propagated to the far field in a consistent way. We demonstrate the effectiveness of this method by modeling the ground motion observed during the Source Physics Experiment. 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-679820

A Theoretical and Computational Setting for a Gradient-enhanced Plasticity Theory : Small and Finite Deformations

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ABSTRACT

In this work, a coupled thermo-mechanical gradient-enhanced continuum plasticity formulation is developed within the thermodynamically consistent framework and corresponding two-dimensional finite element analysis is implemented to examine the micro-mechanical and thermal characteristics of the small-scale metallic volumes based on the small and large deformation theories. In the first part of the work, the theory based on the small deformation is proposed with the concept of thermal activation energy and the dislocations interaction mechanisms. The theory is also based on the decomposition of the thermodynamic microforces into energetic and dissipative counterparts, decomposition of free energy into the elastic, defect and thermal counterparts, and decomposition of dissipation potential into the mechanical and thermal counterparts. The temperature distribution in the system, due to the conversion of the plastic work into heat and the partial dissipation of the heat due to the fast transient time, is included into the model using a generalized heat equation. The derived constitutive model is validated through the comparison with the experimental observations conducted on micro-scale thin films. The proposed model is applied to the simple shear problem and the square plate problem respectively in order to investigate the thermo-mechanical behavior and the grain boundary effect of small-scale metallic materials. In the second part of the work, two-dimensional finite element simulation for the finite deformation incorporating the temperature effect is developed based on the implicit gradient-enhanced approach, F-bar method and radial return algorithm. The implicit gradient approach is well known for its computational strength, however, it is also commonly accepted that it cannot capture the size effect phenomenon observed in the small-scale experiments during the strain hardening regime. In order to resolve this issue, a modified implicit gradient approach which can capture the size effect under the finite deformation is constructed in this work. The simple shear problem is then solved to carry out the feasibility study of the proposed model on the size effect phenomenon. Lastly, the uniaxial plane strain tension problem is solved to perform the mesh sensitivity tests of the model during the strain softening regime.

Polygonal Analysis and Polytree-based Adaptive Topology Optimization of Fluid-submerged Breakwater Interaction

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ABSTRACT

This research presents the application, for the first time, of polygonal finite element method (PFEM) and polytree-based adaptive topology optimization technique to simulate and optimize fluid-submerged breakwater interaction problems. They are integrated to investigate fluid-structure interaction (FSI) problems between fluid and submerged breakwater (SBW). Then an optimal shape of SBW is main goal of this study. In addition, SBW is one of the most interesting protected solution in coastal structures because its distinguished features, particularly, protecting the landside from the erosion without any loss of beach amenity and negative aesthetic influents for the recent decade instead of seawall, groins, breakwater, etc. And It is always subjected the fluid interaction. In this study, some numerical examples are presented to demonstrate the effectiveness of the proposed method. A finite element commercial package, ABAQUS software, is used to produce reference solutions for the numerical examples written in MATLAB.

Plasma Actuators for Flow Control of Flapping Wing

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ABSTRACT

The concept of fixed wing Micro Air Vehicle (MAV) has gained increasing interest over the past few decades, with the principal aim of carrying out surveillance missions. The design of flapping wing MAV is still in the infancy stage. On the other hand, researchers have been increasing interest in dielectric barrier discharge (DBD) plasma actuators for active flow control over ten years. The aim of this study is to investigate the performance of flapping wing MAV using active flow control (i.e. DBD plasma actuators). First, a study of a NACA 0012 airfoil will be performed for the aim of improving its aerodynamic performance with particular focus on the lift over drag coefficient. The fluid-structure interaction will be studied to show the versatility of DBD plasma actuators. The benchmark case will be validated with published literature. For the plasma-fluid interaction, we will use reduced-order model to solve plasma induced electric body force. The OpenFOAM CFD platform will be used to solve the problem. For the plasma induced turbulence in the flow regime, $k-\epsilon$ turbulence model will be adopted to address the interaction between plasma and fluid flows. In future, the combination of the flapping wing design with DBD plasma actuators would boast a maneuverability of MAV.

Cyclic Pseudoelasticity of Polycrystalline Shape Memory Alloys: Constitutive Modeling and Numerical Simulation

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ABSTRACT

This work presents a new 3D thermomechanical finite-strain constitutive model for cyclic pseudoelasticity of polycrystalline shape memory alloys (SMAs). The model considers four primary characteristics related to the cyclic behavior of SMA that have not been integrally addressed within the finite-strain framework: (i) large accumulated residual strain that results from the residual martensite and dislocations slipping during cycling; (ii) degeneration of pseudoelasticity and hysteresis loop due to the increase of dislocation density and internal stresses with the number of cycles; (iii) rate dependence that can be attributed to the thermomechanical coupling effect; (iv) evolution of the phase transformation from abrupt to smooth transition, as a consequence of the diversified crystallographic orientations of the grains, the heterogeneity of internal stresses, and the presence of non-transforming precipitates during cycling. Based on the decomposition of finite Hencky strain into elastic, transformation, residual and thermal components, the model is constructed within a thermodynamically consistent framework. Evolution equations associated with the internal variables are derived from the reduced form of energy balance, the Clausius-Duhem form of entropy inequality, and a Helmholtz free energy function that includes elastic, thermal, interaction and constraint energies. The model is used to simulate the cyclic tensile experiments on NiTi wire at different loading rates. The good agreement of the model predictions against the experimental data demonstrates the capabilities of the proposed model to well describe cyclic pseudoelasticity of polycrystalline SMAs, and to capture the aforementioned characteristics. Furthermore, in order to demonstrate the capability of the cyclic model to solve multi-axial problems, a finite elements simulation of a SMA torsion spring undergoing large strains and rotations resulting in local multi-axial non-proportional stress and strain evolution is performed.

Structural Optimization Design Method Considering SLM Manufacturing Constraints

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ABSTRACT

SLM (Selective Laser Melting) is one of the most widely used metal AM (additive manufacturing) technologies which is able to manufacture metal components with complex geometries, and shorten the processing cycle. In the manufacturing process of SLM, the manufacturing abilities and parameters has a great effect on the mechanical properties of components. To design the structures meeting the manufacturing abilities, this paper presents a structural optimization design method with considering manufacturing constraints of SLM, to design components can be manufactured without the use of support material. The relationship between the limit height and angle of overhang when the component collapses is studied experimentally, the results of which is used to compose the corresponding self-supporting constraints embedded within the topology optimization framework. The optimized structures is manufactured via SLM technology to verify the effectiveness and correctness of the proposed method and manufacturing constraints.

Impact Characteristics Analysis and Fatigue Life Estimation of Recoil Spring

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ABSTRACT

On automatic or semi-automatic guns, the recoil spring slows the rearward movement of the bolt moving components and pushes it back to the front, which is generally cylindrical helical compressing spring, with a single wire or three, four wire twisted cable. The recoil spring is mainly subjected to high speed impact load in the reciprocating movement. The spring deformation is very fast, and the deformation and stress distribution are very uneven. After long firing, the free length of spring can be shortened, the spring force is weakened and sometimes even fatigue crack or fracture can be produced. The failure of the spring will cause the action of automation to be fatigue and not in place, which will affect the firing accuracy. Therefore, the recoil spring impact characteristic analysis and fatigue life estimation is crucial. In this paper, the finite element simulation method was used to study the impact characteristics of the recoil spring and its fatigue life estimation method. Aimed at the 59 type 12.7 mm airborne machine gun, the dynamic response characteristics of the three-strand recoil spring under the impact of the bolt was analyzed with ABAQUS software, and the time history curve of the stress of the dangerous position was obtained. Then the curve was counted by the rain flow counting method to get the fatigue stress spectrum of recoil spring. According to the Miner damage theory, the fatigue life of the recoil spring was finally estimated based on the fatigue stress spectrum and the S-N curve of the spring material. The results show that the recoil spring has obvious transient in the impact process of the bolt, the impact velocity is far greater than the internal stress wave propagation speed of the spring, which is easy to make spring rings to merge together. And the stress wave is not reflected at the fixed end of the recoil spring during propagation, the maximum stress appears at the fixed end of the spring. Using the median fatigue curve (survival rate 50%), the estimated fatigue life of the recoil spring is about 6000 times, which is consistent with the overall life of the whole gun. The method presented in the paper can provide technical means for the fatigue life prediction and parameters design of multi-strand spring.

Barycentric Stencils

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ABSTRACT

Dirichlet kernels provide a tool for analytic construction of harmonic barycentric coordinates (piecewise linear on the boundary) over any C^1 bounded region¹. These may be approximated well by more easily computed corresponding coordinates for inscribed polygons. A simple stencil is a ring with inner boundary the C^1 curve and outer boundary a similar curve or convex polygon. When the outer boundary is also a C^1 curve and a $C^?$ approximation is required within the ring, the Dirichlet barycentrics extrapolate into the ring while the polygon coordinates do not. Numerical studies with inner and outer ellipses are described. 1. Eugene Wachspress, Rational Bases and Generalized Barycentrics, Springer, 2016, pp 228-232

Phase-field Study of Dendritic Growth of Hexagonal Crystal in Thin Film

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ABSTRACT

Hot-dip galvanizing is a coating process to prevent steel from corrosion. In the process of hot-dip galvanizing, a steel material is immersed in a liquid bath of a molten zinc alloy, and the coating layer is formed through solidification. Then, very large grains with a (0001) orientation, termed spangles, are preferentially formed in the coating layer. Although it was reported that the (0001) texture of the coating layer was formed by a preferred (0001) nucleus orientation and preferential dendrite growth in a basal plane [A. Sémoroz et al., Metall. Mater. Trans. A, 33 (2002) 2695-2701], the detail morphological evolution and dendrite growth kinetics of the dendrite in such thin layer are not clear even now. In this study, we investigate the formation mechanism of the (0001) texture by performing dendrite growth simulations of a hexagonal crystal in thin film using a phase-field method, which is well accepted as the most accurate dendrite prediction model. Here, the phase-field simulations are systematically performed in the two- and three-dimensions by changing the crystal orientation and wetting angle between the dendrite and substrate surface. The dendrite growth velocity and morphology are investigated in detail.

Fundamental Study for Crack Propagation Forecast Using Machine Learning

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ABSTRACT

This paper presents the capability and applicability for fatigue crack propagation evaluation using a neural network system. Fatigue crack propagation includes several governing laws and computation methods which are elastic stress field, stress intensity factors, Paris's law, criterion of crack propagation direction. Crack propagation phenomenon simultaneously occurs with these laws and methods. In this paper, we compute crack propagation as training data in 2-dimension using s-version finite element method. Three training levels are defined. In 1st training level, crack position vector, propagation direction vector and stress intensity factors are learned. In 2nd training level, crack position vector, crack propagation direction vector, six stress components around crack tip are learned. In last training level, only crack position vector and crack propagation direction vector are trained. Last level requires only geometrical information to predict crack propagation phenomenon. In order to simplify the problem, all of parameters are completely determined as constant values. The simulation can represent curved crack path by incremental crack propagation computations. As a result of comparisons between the each level, the 1st level exhibits the highest reproducibility. If the same computation results as the 1st level, the last level requires 10 times training data and time to get convergence of the neural network system. We'd like to discuss the results of several learning examples and show the applicability of the neural network technology to the actual engineering problems.

Uncertainty Quantification of Data Collection and Data Processing in Materials Characterization

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ABSTRACT

Serial sectioning techniques for the development of three dimensional microstructures are important to the advancement of material behavior modeling. Three dimensional microstructures provide valuable statistical information about the underlying structure and defects of a given material sample. However, due to the nature of serial sectioning techniques the material sample is destroyed in the process, and such methods often provide no quantitative measure of the accuracy to which they represent a physical sample as a digital microstructure. Furthermore, serial sectioning data sets are expensive in terms of time and resource allocation, meaning that error estimates based on analysis of multiple larger scale experiments is prohibitive. Without such measures of accuracy, error propagates unaccountably to material modeling and simulation experiments. To address the issues of error propagation, and experimental accuracy vs. experimental cost, a computational method was developed to simulate serial sectioning data collection. By simulating the data collection process for Electron Backscatter Diffraction (EBSD) and other serial sectioning techniques, the effect of many different experimental parameters can be study with respect to their impact on the total experimental error. User defined parameters such as resolution, slice thickness, dwell time, and polishing method all have a direct correlation to both the accuracy and experimental cost of a given serial sectioned data set. By varying each of these parameters the effects can be studied individually and provide bounds for both individual sources of error as well as the total error introduced through the experiment process. This is done by starting with a digital representation of a material, and simulating serial sectioning data collection on the digital material. The final results can be compared directly to their original source. Thus, providing a quantifiable comparisons of accuracy for different experimental parameters. Finally, this work seeks to demonstrate how each of these errors propagates from the experimental data collection stage through the modeling stage. Finite element simulations of virtually collected data illustrate changes in the final solution variables, and provides estimated bounds of the error introduced by changing different experimental parameters. Ultimately, this work this provides a method to account for inerrant errors of reconstructed microstructures and inform experimentalist on best methods for experimental uncertainty quantification.

Inverse Problems for Smart-City Applications

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ABSTRACT

By 2050, about 75% of the world population would live in cities, despite the fact that most of the urbanites actually complain about their quality of life in cities, especially concerning the air pollution, the mobility/congestion and the thermal comfort in bad insulated buildings. Through the concept of Smart-City, by combining innovative sensors and new numerical technologies, new services can be proposed to the urbanites to facilitate their day-to-day living and new tools can be provided to the territorial collectivities to manage the cities. In addition, virtual testing and simulation can help selecting optimal urban plannings to move towards efficient, sustainable and green cities. In the presentation, we focus on the utility of inverse problems coupling sensor outputs and physical model for Smart-City applications. Firstly because of the costliness of some sensors, such as gaz sensor for air quality monitoring, their number and placement have to be optimized. In [1], we proposed an adjoint-based tool to evaluate the observability area associated to a given sensor position. Thus, air/water quality sensors can be optimally placed to localize indoor source emissions or to detect contaminants in drinking water networks. Then, the updating of model parameters by solving inverse problems can be of interest to reconstruct fields, like the flow in drinking water networks [2] for leak detection, and to monitor structures, like the localization and the quantification of damage in concrete structures [3] and in-situ evaluations of wall thermal resistance before and after rehabilitation works. Lastly, a new inverse problem formulation is presented to precisely predict quantities of interest and is applied to thermal building problems. Some of these experiments were conducted in the French equipment "Sense-City". [1] J. WAEYTENS, P. CHATELLIER, F. BOURQUIN, 2013, Sensitivity of inverse advection-diffusion-reaction to flow, sensor and control: a low computational cost tool, *Computers & Mathematics with Applications*, 66, 1082--1103. [2] J. WAEYTENS, P. CHATELLIER, F. BOURQUIN, 2015, Inverse Computational Fluid Dynamics: Influence of Discretization and Model Errors on Flows in Water Network Including Junctions, *Fluids Engineering*, 137 (9), 17p. [3] J. WAEYTENS, B. ROSIC, P-E. CHARBONNEL, E. MERLIOT, D. SIEGERT, X. CHAPELEAU, R. VIDAL, V. le CORVEC, L.-M. COTTINEAU, 2016, Model updating techniques for damage detection in concrete beam using optical fiber strain measurement device, *Engineering Structures*, 129, 2--10.

Multiscale Process-Structure Simulation for Additive Manufacturing in Metals Using a Cellular Automaton Model

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ABSTRACT

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.

Model-Based Control of Integrated Fluidic Actuators for Adaptive Structures

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ABSTRACT

Adaptive structures in structural engineering include sensors and actuators to influence the systems' response under stationary and dynamic loads. The induced structural stresses and displacements can be compensated by stationary adaption and dynamic control [1]. To provide a high integration level of the active elements, a new kind of fluidic actuator is developed. As proof of concept, a concrete beam is equipped with hydraulic pressure chambers which are arranged asymmetrical regarding the neutral axis. Thus the beam's deflection can be changed actively to reduce load induced displacements and achieve a more homogeneous stress distribution. In this work, a continuous model of the integrated fluidic actuator is formulated by means of a partial differential equation, based on the Euler-Bernoulli beam theory. The right hand side of the equation is realized using spatial characteristics in combination with time-dependent inputs. For this actuator, a control law is derived based on the equations of motion with the aim of controlling the deflection curve or the boundary forces and torques. We show that the derived model can also be used to find optimal actuator configurations in terms of geometry and position of the integrated pressure chambers [2]. Furthermore, both the controller design and actuator design problem can be combined in a holistic approach. The controller's effectiveness and the systems performance are shown by means of numerical results. [1] W. Sobek and P. Teuffel, "Adaptive systems in architecture and structural engineering," Proceedings of SPIE, vol. 4330, 2001, pp. 36–45. [2] M. Heidingsfeld, P. Rapp, M. Böhm, and O. Sawodny, "Gramian-based actuator placement with spillover reduction for active damping of adaptive structures," Proceedings of the 2017 IEEE/ASME International Conference on Advanced Intelligent Mechatronics (AIM 2017), 2017.

High Reynolds Aerothermal Simulations and Reduced Basis in Feel++

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ABSTRACT

We present in this talk our work on model order reduction for aero-thermal simulations. The model involves the resolution of coupled non-linear parametrized partial differential equations in which affine decomposition is not obtained. We consider the coupling between the incompressible Navier-Stokes equations and an advection diffusion equation for the temperature. Since the physical parameters induce high Reynolds and Peclet numbers, we have to introduce stabilisation operators in the discrete formulation in order to deal with the well known numerical stability issue. The chosen stabilization, applied to both fluid and heat equations, is the usual Streamline-Upwind/Petrov-Galerkin (SUPG). This method often produces non physical undershoots or overshoots in the edge of discontinuities, which can be critical. To tackle this discontinuity problem, we add in our model a new operator, known in the literature as shock capturing method. This new operator is non-linear and adds artificial diffusivity in the region of the discontinuities in order to treat under/overshoots. Although this method is particularly efficient, it induces a new difficulty, because the system becomes fully non-linear. We present in this talk our order reduction strategy for this model, based on Reduced Basis Method (RBM). In order to recover an affine decomposition for this complex model, we implemented a discrete variation of the Empirical Interpolation Method (EIM) which is a discrete version of the original EIM. This variant allows to build an approximated affine decomposition for complex operators such as in the case of SUPG. We also use this method for the non-linear operators induced by the shock capturing method. The construction of an EIM basis for non-linear operators, involves a potentially huge number of non-linear FEM resolutions - depending on the size of the sampling. Even if this basis is built during an offline phase, we usually cannot afford such expensive computational cost. We took advantage of the recent development of the Simultaneous EIM Reduced basis algorithm (SER) to tackle this issue. Enjoying the efficiency offered by reduced basis approximation, this method provides a huge computational gain and can require as little as $N+1$ finite element solves where N is the dimension of the RB approximation. As an illustration we present an application of a cooling system of a printed circuit board with different heat sources. The model is parametrized with different physical and geometrical parameters. This work has been funded by the ANR project CHORUS.

MATHEMATICAL AND COMPUTATIONAL MODELING FOR STUDYING THE VIBRATION OF A BEAM WITH MODIFIED STIFFNESS

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Key Words: Mathematical Analysis, Computational Modeling, Modified Stiffness, Vibration, Support of Machine.

Abstract: Vibration analysis is of extreme importance in industrial projects involving rotating machines and their supports. Vibration is an effect that reduces the accuracy of assembly systems, results in loss of production quality, increases the need for maintenance, generates excessive noise, as well as putting the health and safety of workers at risk. Almost all industrial divisions are subject to this problem. The dynamic characteristics of structures are known to depend on their stiffness and mass; these are key parameters in determining natural frequencies and modes of vibration. However, the initial stiffness of a structural system, calculated in its unloaded state, can be affected once loading forces are applied; this constitutes the so-called geometric stiffness. Mathematical analysis and computational modeling were performed to evaluate the influence of geometric stiffness on the fundamental frequency of a support system. The former provides a practical and efficient equation for calculating the altered system frequency. The latter allows the inclusion of elements that make it a sophisticated instrument in the search for solutions, thereby increasing the capacity of analysis. The mathematical analysis utilizes a model based on the Rayleigh method, which was developed to represent a beam with simple supports designed to function during periodic excitation. In this case, a compressive force reproduces the effects of a horizontal load, which alters the stiffness and consequently the natural vibrational frequency of the structure. Computational modeling, in turn, is constructed at different hierarchical levels using the finite element method. As the hierarchy of the models increases, more details can be incorporated, approaching the physical problem at ever higher levels of fidelity and with the possibility of incorporating structural components. This would not be possible in the most basic models. The results point to a close approximation between the mathematical solution and the various levels of computational modeling, with differences of less than 2%.

1. INTRODUCTION

Dynamic characteristics of a structure essentially depend on its stiffness and mass. Through these two elements, the natural frequencies and modes of vibration of the system are determined. However, the initial stiffness of a structure, as demonstrated in the unloaded state, is affected by the presence of loads, producing the so-called geometric stiffness (see ^{[1]-[6]}). This is the case for compressive loads. Brought to its limit, this decrease may lead to system instability.

Machine bases are an economically and strategically vital subset of national industry. They are subject to vibrations induced by the supported equipment. These vibrations can affect the safety of the structure and generate effects harmful to the equipment and detrimental to the quality of the product manufactured. They can also make the work environment unsafe. Moreover, the value of equipment commonly exceeds the value of support structures, both in terms of replacement costs, as well as due to incurred costs of downtime when operations must be suspended.

In particular, the model that was analyzed in this work represents a machine base composed of a steel pinned-roller beam simulating a rotary machine support. The presence of a normal compression force acting on the structural system decreases the stiffness of the beam and consequently its natural frequencies of vibration; this can lead to unexpected resonance regimes depending on the engine operating frequency. For this reason, the effects of loading on the stiffness of a beam as support were studied numerically by an exact mathematical solution and computational modeling.

2. MATHEMATICAL SOLUTION

From a dynamics point of view, a beam is a continuous system with infinite degrees of freedom. In many cases, a practical way of studying the beam motion is to associate it with a system possessing a single degree of freedom (SDOF). To do this, a certain function is assumed to ideally reproduce the desired form of vibration to study by applying it to the generalized coordinate, which is conveniently chosen to represent the oscillatory movement amplitude.

Thus, after deliberate study, the frequency can be found by equating the maximum strain energy developed during the motion with the maximum kinetic energy. The use of a function as previously mentioned was presented by Rayleigh^[7] in 1877 for studying vibration in mechanical systems. The concept behind this method is the conservation of energy principle, which can be applied not only to systems with a finite number of degrees of freedom but also to continuous systems for determining the fundamental period of vibration.

Consider a rotary machine mounted on a beam subjected to a compressive force. It is known that such forces affect the geometric stiffness and thus the values of the undamped free vibration frequencies. Designing the structure to possess frequencies that exceed the machine's service speed rotation may make it vulnerable to potentially dangerous resonance conditions due to geometric stiffness from frequency changes.

Assume Bernoulli-Euler beam theory for the following system (Figure 1). A support beam AB of length L and inertia I functions as the base to an engine E_g , which consists of linear elastic material that is represented by the modulus of elasticity E . A normal force of compression P

reproduces the force that changes the stiffness and consequently the natural frequency of vibration of the structure f_n . The eccentricity between the engine axis and the part is initially ignored. The vertical displacement of the central joint is the generalized coordinate of the system. By using the Rayleigh method, the undamped vibration frequency in its first mode is obtained.

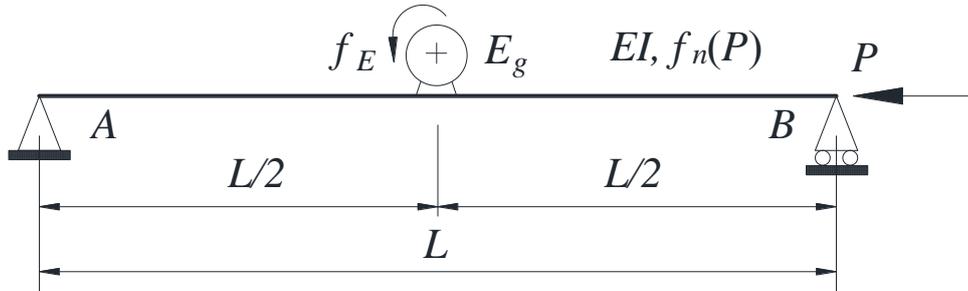


Figure 1. Beam as the base of an engine.

Consider also that the vertical displacement of a generic section of the beam in Figure 2 is given by

$$v(x, t) = \phi(x) q(t), \quad (1)$$

in which $\phi(x)$ is a shape function that attempts to define the boundary conditions in the supports and value 1 in the central section of the beam, whose displacement with time is $q(t)$.

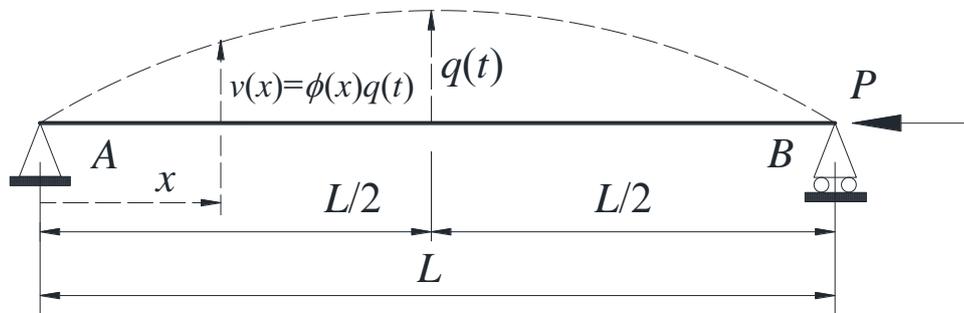


Figure 2. SDOF mathematical model of vibration.

In this case, one adopts the shape function given by Eq. (2):

$$\phi(x) = \sin\left(\frac{\pi x}{L}\right), \quad (2)$$

which is the exact solution of the problem without the P load. A prime mark will denote a derivative of the function in relation to x .

Applying the Rayleigh method, one has the conventional bending stiffness, K_0 , as a function of the material elasticity and the geometry of the cross, which is equivalent to

$$K_0 = \int_0^L EI (\phi'')^2 dx, \quad (3)$$

where EI is the known flexural bending, which is represented by multiplication of the material modulus of elasticity with the inertia of the section in relation to the the vertical vibration mode. In turn, the geometric stiffness, K_G , as a function of the normal force of compression is equivalent to:

$$K_G(P) = P \int_0^L (\phi')^2 dx. \quad (4)$$

The total generalized mass of the system is found by calculating

$$M = M_C + M_V \quad (5)$$

where M_C is the concentrated mass at the middle span and M_V is the mass coming from the beam self-weight given by

$$M_V = \int_0^L m_V \phi(x)^2 dx, \quad (6)$$

in which m_V represents the mass per length unit. Finally, the frequency of undamped free vibration (in rad/s) is found by way of Eq. (7):

$$\omega(P) = \sqrt{\frac{K(P)}{M}}. \quad (7)$$

Considering the total beam stiffness as a function of P given by

$$K(P) = K_0 - K_G(P), \quad (8)$$

the free undamped frequency of vibration of the 1st mode is found, in Hertz, admitting the compressive force as positive, by:

$$f_n(P) = \frac{\omega(P)}{2\pi} = \frac{1}{2} \left[\frac{\pi^2 EI - PL^2}{L^3 (L m_V + 2M_C)} \right]^{\frac{1}{2}}. \quad (9)$$

The effects of geometric stiffness can be realized by considering a simple supported beam with theoretical length L equal to 2 m and cross-section as defined in Figure 3, where t is the thickness of the wall and h is the external side dimension of the square section adopted. The adopted dimensions of the beam are: $h = 50$ mm, $t = 1.5$ mm.

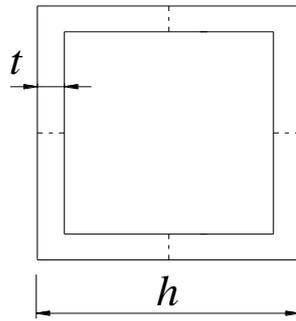


Figure 3. Adopted cross-section.

When considering Figure 4, it is observed that the presence of the compressive force P truly reduces the beam stiffness and consequently its natural frequencies $f_n(P)$. If the engine operating frequency intercepts $f_n(P)$, it could lead to unexpected and potentially dangerous resonance regimes during operation.

The natural frequency of the beam has been calculated by using Eq. (9), taking a density of the material of 7850 kg/m^3 , a lumped mass at the central position of the span (engine mass) equal to 4.6 kg , and a modulus of elasticity of 205 GPa .

3. COMPUTATIONAL MODELING

Concerning the mathematical procedure, the formulation corresponding to the finite element method (FEM) is performed by finding the eigenvalues and eigenvectors by Eq.(10)

$$\{[K] - \omega^2 [M]\} \Phi = 0, \quad (10)$$

where $[M]$ is the mass matrix, and $[K]$ is the stiffness matrix, which for the geometric non-linear case includes the parcel of the geometric stiffness, configuring a similar formulation to that described in Eq.(8). The matrices in Eq.(10) for the different types of modeling can be found in Cook^[8].

The computational modeling as exemplified in Figure 4 was constructed in ANSYS Academic Version at different hierarchical levels of complexity with respect to the physics of the problem. Such modeling was based on the modified stiffness of the beam from a previous non-linear static analysis with the inclusion of the geometric stiffness parcel to obtain the total stiffness of the base, as described previously. This means that the stiffness matrix obtained at the end of the static processing was used to calculate the frequency of the first mode of vibration. A Poisson coefficient of 0.3 was added to the data described in the previous item.

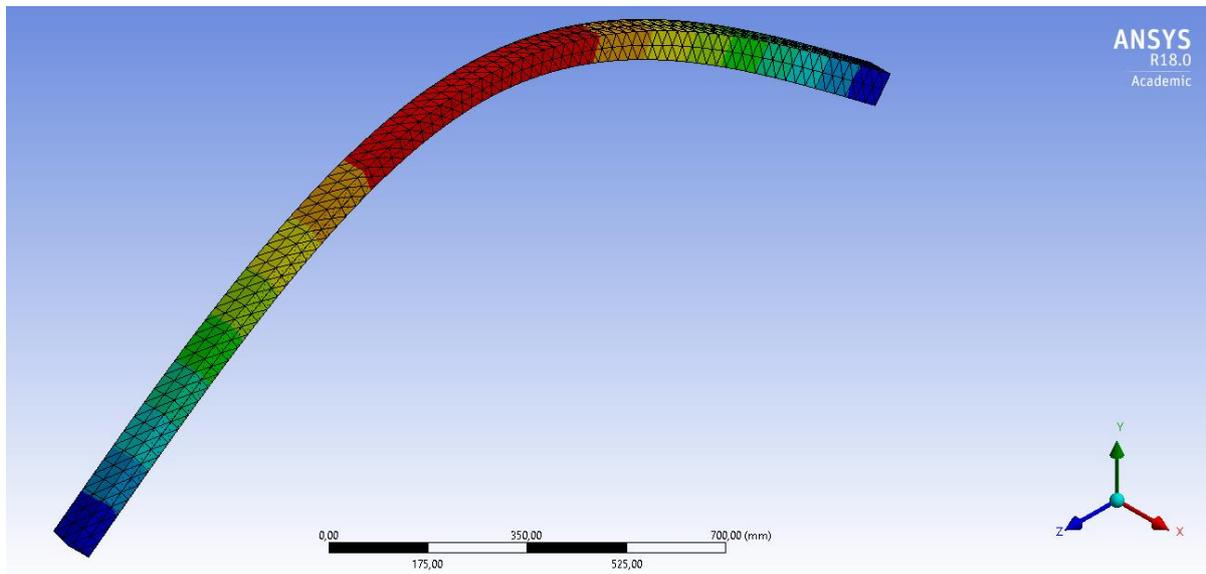


Figure 4. Computational model by FEM.

Three computational models were developed for studying the system at hierarchically increasing levels of complexity with respect to computational modeling: FEM 1D (unidimensional model with frame elements), FEM 2D (two-dimensional model with shell elements) and FEM 3D (tridimensional model with solid elements). The models are differentiated by the computational cost required for the finite element types used and by the possibility of generating more accurate results.

Moreover, as the hierarchy of models advances, more detail can be incorporated to approach the physical problem at ever higher fidelity levels and with the possibility of incorporating different structural components, which in the most basic models would not be possible. The models were elaborated according to the geometry defined for the mathematical simulation. The program was executed for the three hierarchical levels, thus making it possible to compare the results obtained with the analytical result as depicted in Figure 5.

As can be observed, the results generated in the computational modeling are adequate for the mathematical solution presented in Eq.(7), with an average difference of 1.5% between them. It should be noted that the FEM 3D model is the most complete and complex of all the models. For the 3D model, when the force reaches values close to 54 kN (near the collapse) a difference of 11.44% is found. This relates to the non-linear characteristic of the problem due to the internal stress level, which elevates the sensitivity of the model to the discretization used. It should be mentioned that this aspect was studied by Wahrhaftig^[9] who found in a similar context, a difference of up to 21% in the analyses performed (linear and non-linear).

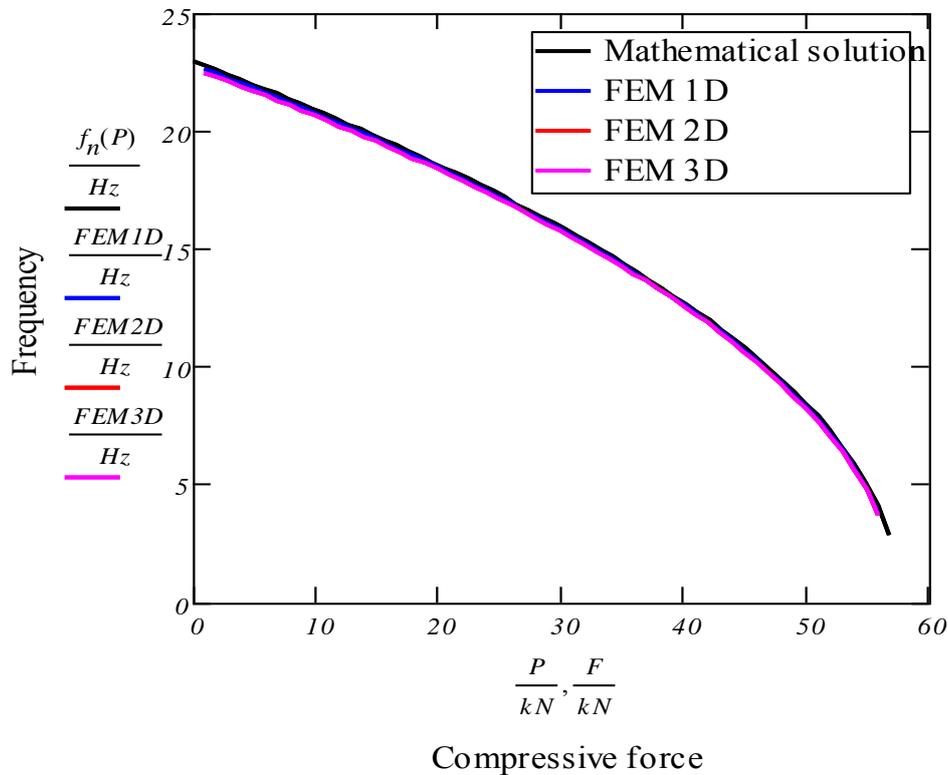


Figure 5. Comparison of results.

4. ACKNOWLEDGEMENT

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5. CONCLUSION

- A vibration study of a beam with its stiffness geometrically altered was detailed by theoretical-analytical analysis and numerical-computational models.
- A model of a metallic pinned-roller beam operating under the effect of axial compression loads was elaborated upon to analyze the variation in its fundamental frequency while considering the applied forces.
- The effect on the geometric stiffness which is influenced by the horizontal loading and the corresponding possibility of introducing resonant regimes in the structural support system were demonstrated by calculating their frequencies.
- According to theory, increasing the axial compressive force can induce resonance conditions to manifest.
- In summary, it is possible to affirm that computational modeling yields a good approximation to the mathematical solution developed in this work.

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Free-form Optimization Method for Controlling Transient Response of a Linear Elastic Structure under Dynamic Loadings

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ABSTRACT

Many natural vibration and frequency response problems were solved under the assumption of the harmonic vibration and the optimization methods for these two problems have been studied in many previous works because of the easy handling and conventionality. On the contrary, we propose a non-parametric shape optimization method to control the transient response of a linear elastic structure in this study. The estimation of the real response under the transient load is essential in the design of vehicles or structure under seismic loadings, where the loadings act dynamically, non-harmonically. We consider the viscous damping and the transient forced loads or the impulse loads are applied. In the development of the non-parametric shape optimization method, the free-form optimization method with H1 gradient method, is applied to the transient response problem. The design objective is to minimize the dynamic compliance, which is defined as the time integration of the each discretized time's compliance or to control the amplitude at arbitrary domains and times to the desired values. In these two optimization problems, the linear transient response is directly solved without converting the equivalent static loads method, which is often employed in the time-dependent non-linear optimization problems. The optimum design problems are formulated as a distributed-parameter optimization problem and the sensitivity functions for both optimization problems are theoretically derived using the material derivative and the adjoint methods. The derived sensitivity function is applied to the H1 gradient method to determine the optimal shape variation. With this method we can obtain the optimal free-form shape that reduces the objective functions while maintaining the surface smoothness. The some optimum design examples are demonstrated to show the effectiveness of the proposed method and the results are discussed.

Adjoint Based Data Assimilation for Quantification of Dynamic Mechanical Behavior of the Heart

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ABSTRACT

Accurate biophysical models offer promise for improved understanding of cardiac functionality. However, the myocardium is a complex dynamic material, and while detailed models and constitutive laws describe its passive and active behaviour, fitting these models meaningfully to actual data is greatly complicated by the large number, and interaction of, required parameters. Although numerous techniques, from trial and error to advanced optimization, can be used to fit data, challenges still exist, often due to the computational requirements to search for optima. This is particularly challenging when considering real observations, where heterogeneous noisy data sets are the norm, and time constraints are present. Here we discuss the use of adjoint methods as an attractive, efficient means to rapidly assimilate large data sets into personalized models of cardiac mechanics. These optimization techniques allow us to fit models at a cost that does not significantly depend upon the numbers of parameters to be fit, and thereby provide an excellent means to assimilate high dimensional parameter spaces at a relatively low computational cost. These methods are enabled by the new generation of software tools that automatically create physical models and derive adjoint equations for problems of interest.[1,2] We describe the methodology, and show the utility of this method in a range of clinically driven applications.[2,3] In all these cases, we use an efficient pipeline to create cardiac models directly from medical imaging and applied adjoint based PDE constrained optimization to assimilate dynamic geometric information into fit models. These rapidly produced parameterized mechanical models demonstrate differences in active and passive properties of the myocardium in disease states, which may have diagnostic use as biomarkers. Reducing the computational cost of accurate models is a key step towards translating into greater utility, both for basic science and for eventual clinical adoption. We show that adjoint based PDE constrained optimization methods, and in particular their applicability for data assimilation, offer the means to accelerate the use of biophysical models. [1] Logg, A. et al. The FEniCS book (Vol. 84), 2012 [2] Farrell PE et al. Automated derivation of the adjoint of high-level transient finite element programs. SIAM Journal on Scientific Computing, 2013. [3] Balaban G et al. High resolution data assimilation of cardiac mechanics. International journal for numerical methods in biomedical engineering, 2017. [4] Finsberg et al. Estimating cardiac contraction through high resolution data assimilation of a personalized mechanical model. Journal of Computational Science, 2017.

An Improved Contact Method for Multi-material Eulerian Hydrocodes

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ABSTRACT

Realistic and accurate modeling of contact for problems involving large deformations and severe distortions presents a host of computational challenges. Due to their natural description of surfaces, Lagrangian finite element methods are traditionally used for problems involving sliding contact. However, problems such as those involving ballistic penetrations, blast-structure interactions, and vehicular crash dynamics, can result in elements developing large aspect ratios, twisting, or even inverting. For this reason, Eulerian, and by extension Arbitrary Lagrangian-Eulerian (ALE), methods have become popular. However, additional complexities arise when these methods permit multiple materials to occupy a single finite element. Multi-material Eulerian formulations in computational structural mechanics are traditionally approached using mixed-element thermodynamic and constitutive models. These traditional approaches treat discontinuous pressure and stress fields that exist in elements with material interfaces by using a single approximated pressure and stress field. However, this approximation often has little basis in the physics taking place at the contact boundary and can easily lead to unphysical behavior. This work presents a significant departure from traditional Eulerian contact models by solving the conservation equations separately for each material and then imposing inequality constraints associated with contact to the solutions for each material with the appropriate tractions included. The advantages of this method have been demonstrated with several computational examples. This work concludes by drawing a comparison between the method put forth in this work and traditional treatment of multi-material contact in Eulerian methods.

Numerical Study of Effect of KC Number on the Vortex-Induced Vibration of a Flexible Riser in the Oscillatory Flow

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ABSTRACT

In offshore oil and gas drilling, relative oscillatory flow is generated between the platform and the riser by the effect of wind, waves and currents. The riser in the deep-water not only bears the weight and the top tension, but its amplitude increases obviously when the vortex shedding frequency is close to the natural frequency of the riser which does harm to the safety of the platform. So the study of Vortex-induced vibration (VIV) of an isolated riser in relative oscillatory flow is necessary to prevent the fatigue damage of the platform structure. In this paper, numerical simulations are carried out by our in-house CFD code viv-FOAM-SJTU, which is developed based on the open source code OpenFOAM. The strip theory and the Reynolds Averaged Navier-Stokes(RANS) equations are used to analyze the flow field. The Bernoulli-Euler beam theory with the FEM method is used to obtain the structural dynamics response. The oscillatory flow is simulated by forced excitation added at both ends. To achieve the fluid-structure interaction, interpolation module is developed to transmit data between the fluid and structure model. In this paper, numerical simulation of a flexible riser is carried out at first. Results are compared with the model test to verify the validity of the solver. Then, cases with different motion amplitudes and the same KC number are presented. Diameters of the cylinder change to assure the same KC number. Mechanism of the vibration are articulated through modal decomposition and wavelet transformation. Finally, cases with different KC number with the same motion amplitudes are simulated to explain the effect of KC number in the VIV of the riser in the oscillatory flow. Typical characteristics of the vibration are observed including the modal transition and the "build-up-lock-in-die-out" process.

A Matlab Tool for Scalable Uncertainty Evaluation and Its Use in Optimal Control

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ABSTRACT

Dynamical systems often operate in uncertain environments, which modulate the systems' dynamics and complicate the system analysis and control tasks. These uncertainties often possess the following features: 1) some of their statistical information can be obtained from environmental forecasting tools, 2) they are of high dimensionality, and 3) they cannot be represented by simple Gaussian noises, and 4) they modulate system dynamics in a nonlinear fashion. A critical step in the optimal control of these dynamical systems involves the evaluation of system output statistics under such uncertainties. Monte Carlo simulation and its variants have been used. However, they run into high computational load due to the nonlinear modulation of high dimensional uncertainties. We develop a Matlab tool for uncertainty evaluation, based on a method that we recently developed, called M-PCM-OFFD. As we have proven in [1,2], M-PCM-OFFD integrates the Multivariate Probabilistic Collocation Method (PCM) and Orthogonal Fractional Factorial Design (OFFD) procedures to achieve an accurate, robust, and scalable uncertainty evaluation performance. The Matlab tool takes the number of uncertain parameters, their statistical information, and the simulation model as inputs, and automatically generates a low-order approximated simulation model and estimated output statistics. In the presentation, we will illustrate the principles of the M-PCM-OFFD method, and then describe how the Matlab tool operates. We will also demonstrate how this tool can be used to solve practical optimal control and reinforcement-learning based control problems [3]. The tool and its supporting methodology contribute to the field by providing additional performance insights of OFFD and by, for the first time, bringing OFFD online to solve automatically uncertainty evaluation and optimal control problems. References: [1] J. Xie, Y. Wan, Y. Zhou, K. Mills, J. J. Filliben, Y. Lei, and Z. Lin, "Effective and Scalable Uncertainty Evaluation for Large-Scale Complex System Applications," in Proceedings of the 2014 Winter Simulation Conference, Savannah, GA, December 7-10, 2014. Journal version under review. [2] J. Xie, Y. Wan, Y. Zhou, K. Mills, J. J. Filliben, and Y. Lei, Effective Uncertainty Evaluation in Large-Scale Systems (book chapter), Principles of Cyber-Physical Systems, edited by S. Roy and S. Das, Cambridge University Press, in press, pp. 1-25, 2016. [3] J. Xie, K. Mills, J. J. Filliben, F. L. Lewis, "A Scalable Sampling Method to High-dimensional Uncertainties for Optimal and Reinforcement Learning-based Controls," IEEE Control Systems Letters, Vol. 1, No. 1, pp. 98-103, July 2017.

Mapped Finite Element Method for the Phase Field Approach to Fracture

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ABSTRACT

The phase field method to fracture has attracted widespread attention due to its ability to simulate crack initiation, propagation, merging and branching without extra criteria. However, the singularity around the crack tip deteriorates the convergence property of the method, just like the case of a discrete crack method. In this work, we apply the mapped finite element method proposed by Chiaramonte et al. [International Journal for Numerical Methods in Engineering, 111 (9) (2017) 864-900] to the phase field approach to fracture to attempt to recover the convergence property. The method is based on approximating a much smoother function in a parameterized domain by mapping the solution around the singularity. This reparameterized solution can be well approximated by the finite element method. With a parameter appropriately chosen, the finite element method can achieve an optimal convergence rate for any given order of interpolating polynomials. As the phase field evolves, our method is able to update the center of mapping, presumably the location of the singularity, allowing simulating crack propagation.

A Smoothed Implicit Material Point Method for Geotechnical Applications

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ABSTRACT

This paper presents a novel implicit material point method (MPM), where its formulations and numerical evaluations are detailed. On basis of the partition of unity (PU) concept, the shape functions from the classical finite element method (FEM) are used to construct the PU, while a radial polynomial basis function is employed to construct the nodal approximation. The new formulation synergizes the individual strengths of the traditional FEM and MPM. The inherent stress oscillations in MPM, which is caused by the discontinuities of the shape function gradients between the elements, is greatly improved. Several numerical examples are presented in the paper, including the 1-D bar vibration, 2-D cantilever beam, etc., with the results demonstrating that the proposed smoothed implicit material point method can achieve significantly better accuracy and higher convergence rate, as opposed to the traditional MPM.

A Multiscale Method for Analyzing Progressive Damage of 3D Braided Composite Structure by Using FFT

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ABSTRACT

Abstract: A more efficient multiscale coupling method is developed to study the progressive damage behavior of three dimensional (3D) braided composite structure. In the meso-scale, the fast Fourier transformation (FFT)-based method combining with variational principle is used to overcome the poor convergence for composites with large jumps of material properties. In the macro-scale, the mechanical response of the braided composites is analyzed by using finite element method, in which the stress and stiffness information of each material point can be transformed from the meso-scale results. It is verified that the predicted strength and dominated failure modes of the braided composites structure obtained by the proposed method combining with anisotropic stiffness degradation model are in good agreement with the experimental results. Meanwhile, the high computation efficiency is attractive for large complex structure taking into consideration the nonlinear mechanic behavior. Keywords: Multiscale analysis; Fast Fourier Transforms; Braided composites; Computation efficiency

Theory and Application of Assumed Stress Quasi-conforming Method

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ABSTRACT

Abstract: Quasi-conforming(QC) analysis is a flexible and characteristic finite element method, and the basic idea of the QC method is that the strain-displacement equations are weakened as well as the equilibrium equations. In the QC technique, the element strain fields are approximated using polynomials and integrated using interpolation functions. The assumed stress QC method starts from polynomials approximation of stress and the stress function matrix is chosen as weighted test function to weaken the strain-displacement equations. Unlike the hybrid Trefftz finite element method, the initial approximation of stress is flexible, which can be derived from analytical solutions of equilibrium equations or Taylor expansion. Appropriate approximation of initial stress will make the element formulation simple and concise, and no inner-field functions are needed for the strain integration. The assumed stress QC method has been used for plane stress analysis, couple stress analysis, static and free vibration of Reissner-Mindlin/laminated plates. The constructed elements exhibit advantages of QC technique, free from locking phenomenon and zero-energy modes and insensitive to mesh distortion. The characteristic of boundary integration makes the constructed quadrilateral QC elements can be used to mesh shape degenerates into triangle or concave quadrangle. The method can be generalized for the analysis of trimmed CAD surface in isogeometric analysis(IGA), which also provides an easy way to apply Dirichlet boundary conditions and incorporates IGA with existing finite element codes. Keywords: Quasi-conforming; assumed stress; boundary integration; mesh distortion; isogeometric analysis Reference [1]. Wang CS^{*}, Zhang XK, Hu P. New formulation of quasi-conforming method: A simple membrane element for analysis of planar problems. *European Journal of Mechanics A/Solids*, 2016, 60:122-133. [2]. Wang CS^{*}, Zhang XK, Hu P. A 4-node quasi-conforming quadrilateral element for couple stress theory immune to distorted mesh. *Computers & Structures*, 2016, 175: 52-64. [3]. Wang CS, Wang X, Zhang XK^{*}, Hu P. Assumed stress quasi-conforming technique for static and free vibration analysis of Reissner-Mindlin plates. *International Journal for Numerical Methods in Engineering*, 112: 303-337, 2017.

Sizing and Shape Optimization for Peak Structural Responses under Long-term Processes of Stationary Stochastic Loads

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ABSTRACT

Structural optimization has become a widely used tool to construct efficient structures for various applications due to its capability of providing design freedom and promise for saving material costs. Current optimization methods are usually utilized for optimal structural systems subjected to design constraints under certain definite loading distributions. However, engineering structures experience long-term processes of stationary stochastic loads, owing to various physical environments. In this paper, we develop a novel methodology of structural optimization for peak system responses during long-term processes of stationary stochastic loads. The proposed methodology provides an algorithm for generating structures with the optimal sizes and shapes for constraints on their extreme responses under environmental loads of various statistical features. The computational results confirm that material distribution of optimized structures for peak response constraints highly depends on correlated levels of stationary stochastic loads applied on different spots of the structures under long-term processes. Furthermore, conventional sizing and shape optimization of structures in statics for displacement constraints are also compared with the aforementioned optimized material distribution for peak response constraints under correlated environmental loads. Consequently, the developed methodology provides a powerful tool to investigate efficient structural designs under long-term load processes for fundamental engineering structures and related mechanics researches.

Heaviside Projection Based Aggregation in Stress-constrained Topology Optimization

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ABSTRACT

The presentation introduces an approach to stress constrained topology optimization through Heaviside projection based constraint aggregation. The von Mises yield criterion is adopted to evaluate whether the material fails or not. Our main concern here is on developing a new way to enforce the element-wise local stress constraints. We apply the Heaviside function as an indicator to show the state of the material (safe or failed). If the stress exceeds the yield limit, the indicator function is marked as 1; otherwise 0. Then by integrating the indicator function over the whole design domain and normalizing over the total volume, we obtain the integral of Heaviside projection, which effectively means the volume fraction of the yielded material. As our objective is to make the stress constraint satisfied at every material point, all we need to do is to push the yielded material away, which can be implemented by constraining the Heaviside projection based integral (HPI) to be 0. Based on such Heaviside aggregation, a single global aggregated constraint is constructed. In practice, a smoothed Heaviside function is used as the stress state indicator for differentiability, and a small positive value epsilon rather than 0 is applied to bound the integral. The selection of epsilon is the key to successful enforcement of the stress constraint. If epsilon is too large, the global constraint would not be tight enough to remove the yielded material volume; if epsilon is too small, an over-conservative design would be obtained. In order to get an appropriate threshold epsilon, an adaptive scheme based on the gap between the maximum stress and the prescribed limit is also proposed. As the effectiveness of the global constraint is insensitive to the number of local constraints, this approach is applicable to large scale problems. Our 2D and 3D numerical experiments demonstrate that the single Heaviside aggregated stress constraint can efficiently control the local stress level. Compared to the traditional approaches based on the Kreisselmeier-Steihauser and p-norm aggregations, the Heaviside aggregation based single constraint can substantially reduce computational cost on sensitivity analysis. These advantages make the proposed approach to be applicable to large scale problems.

Topology Optimization of Continuum Structures with Load Position Uncertainty

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ABSTRACT

In the structural design process, not only the structural parameters, such as, the geometry dimensions, material characteristics, boundary constraints, but also the external loads imposed on the structure often have some degrees of uncertainties due to the complicated loading environments. Therefore, in the optimal design of the structural configuration, these uncertainties should be involved properly so as to achieve the efficient load path for the external loads transferring toward the boundaries by allocating the given material more rationally, or for an improvement of the structural performance significantly. In this paper, the topology optimization of a continuum structure with the application position uncertainty of an external force is performed to gain the reliable load paths for transferring the load. Firstly, the position uncertainty of the external load is indicated with the interval variable in accordance with the non-probabilistic approach. Then on the basis of the design sensitivity analysis with respect to the load position movement [1], the structural compliance is expressed as the second-order Taylor series expansion with regard to the position disturbance of the external load. Furthermore, for the computational efficiency, the sensitivities of the structural compliance to the topology design variables are evaluated upon the compliance approximation. Finally, based on the SIMP model and the optimality criteria method [2], the compliance minimization problem is solved readily with consideration of the position uncertainty of the external load, and the numerical results are evaluated in detail against those obtained traditionally under the deterministic load position. Comparisons reveal that the topology optimal designs are obviously different with or without consideration of the load position uncertainty. It will be shown that the obtained topology optimization under consideration is of higher robustness to the disturbances of the load application points since new load paths are often created to accommodate the load position uncertainty.

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Isogeometric Enriched Meshfree Analysis

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ABSTRACT

The B-spline and NURBS basis functions used in isogeometric analysis are naturally convex, which have a variation diminishing property and yield non-negative mass matrices for dynamic analysis. By contrast, the widely used moving least square or reproducing kernel meshfree approximants are non-convex. Thus the construction of convex meshfree approximations is an important recent topic for meshfree methods. The maximum entropy meshfree approximation is a typical convex meshfree approximation, but the extension of this approach to arbitrary order is still an open problem. In this work, the consistency conditions for isogeometric B-spline basis functions and meshfree shape functions are firstly presented in a unified manner. Thus, an isogeometric enriched quasi-convex meshfree method is proposed. The present quasi-convexity of the meshfree approximation is achieved by introducing the mixed reproducing points of isogeometric B-spline basis functions into the meshfree consistency conditions. The resulting meshfree shape functions have an identical form as the standard reproducing kernel meshfree shape functions, while the negative portions of the shape functions are significantly reduced. Consequently, generalization of the proposed formulation to arbitrary higher order basis functions is trivial. It is shown that this isogeometric enriched quasi-convex meshfree method yields better accuracy compared with the conventional meshfree method. The efficacy of the proposed method is demonstrated through several benchmark numerical examples. Key words: Isogeometric analysis; Meshfree method; Consistency condition; Quasi-convex approximation; Mixed reproducing points Acknowledgements: The support of this work by the National Natural Science Foundation of China (11772280, 11472233) and the Natural Science Foundation of Fujian Province of China (2014J06001) is gratefully acknowledged.

Electro-mechanical Characteristics Analysis of Influence Bone Remodeling

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ABSTRACT

The Main factors affecting bone remodeling are bone stress, fluid pressure, fluid shear stress and the streaming potential. In this paper fluid pressure distribution in the bone, fluid shear stress and streaming potential in bone canalicules were studied when bone subjected to dynamic loads. The pore pressure and velocity solutions are obtained to examine the fluid transport behavior and pressure distribution in a loaded osteon on four different exterior surface cases.

The Atomistic Mechanism of Beta Relaxation Processes in Cu50Zr50 Metallic Glasses

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ABSTRACT

It has long been recognized that beta relaxation correlates with numerous mechanical properties of metallic glasses (MGs), while the underlying mechanisms and its structural origin are still under intense debate. In the present study, molecular dynamics simulations were used to examine the beta relaxation of three kinds of atomic structures of Cu50Zr50 MGs, i.e., the materials within and outside of shear band (SB) extracted from the plastically deformed MG, and the as-received MG. Despite their identical compositions, interestingly, the aforementioned MGs exhibit quite different beta relaxation behaviors. Compared to the un-deformed MG with no beta peak, the molecular dynamics simulations results indicated an independent beta peak appeared in the SB like structured specimen, while excess wing corresponding to beta relaxation was observed in the specimen with the deformed non-SB like structure. To the best of the author's knowledge, this is the first time to achieve such dramatic changes of beta relaxation in MGs with identical composition. In addition, the effects of free volume content, shear transformation zone (STZ) size on the quite different beta relaxation behaviors of the three kinds of specimens were characterized. By conducting tensile test via molecular dynamics simulations, the elastic and plastic deformation behaviors corresponding to the various beta relaxations were compared; and furthermore, detailed atomic structural evolution analysis based on the Voronoi polyhedral concept was conducted. The crucial parameters and atomic mechanisms that control the beta relaxation behaviors and mechanical properties of the Cu50Zr50 MGs were suggested and extended discussed. The simulation results presented here provide an in-depth understanding of the structural origin of beta relaxation in metallic glasses and may shed light on the way for synthesizing metallic glasses that could exhibit large tensile plasticity.

Molecular-mechanical Modeling of Fluid Structure at the Solid-fluid Interface and Transport under Nanoconfinement

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ABSTRACT

At the nanoscale, fluids in the vicinity of a solid boundary can arrange in layered structures that exhibit large density inhomogeneities as compared to the bulk fluid (far from the boundary). This effect, which is important for modeling fluid transport at the nanoscale, cannot be described via classical fluid mechanics. In this work, we present several results on mathematical and computational modeling of this layering phenomenon, and in particular the fluid layer directly adjacent to the solid, which we refer to as the first fluid layer. Using Nernst-Planck theory and molecular mechanics arguments we identify a dimensionless group – named the Wall number – that is closely connected with the magnitude of fluid layering at the interface. We also identify and model the relevant lengthscales and density magnitudes of the first fluid layer, such as its distance from the solid boundary, its characteristic width, and its total fluid particle content per unit area, referred to as the areal density. Our modeling results are validated using molecular dynamics simulations for a variety of fluid-solid systems. For the case of dense fluids, we find that the first layer density (defined as the layer areal density divided by its width) scales with the bulk fluid density with a proportionality constant that is only weakly dependent on temperature. Building on these models for interfacial fluid structure, we also present several results connecting fluid layering to anomalous transport under nanoconfinement. In particular, we study the anomalous diffusivity of a fluid confined within a nano-slit. We identify and discuss several key timescales for anomalous diffusive behavior, which are set by the Wall number and the confinement lengthscale. We show that anomalous diffusive behavior of fluid near the solid boundary is due to “dimensional restriction” of this fluid. We demonstrate that the relationship between nanoconfined fluid diffusivity and the confinement lengthscale can be accurately described by averaging the contributions of the bulk and interfacial regions. References: [1] Molecular mechanics and structure of the fluid-solid interface in simple fluids. G. J. Wang and N. G. Hadjiconstantinou. *Physical Review Fluids*, Vol. 2, No. 9, 094201 (2017). [2] Why are Fluid Densities So Low in Carbon Nanotubes? G. J. Wang and N. G. Hadjiconstantinou. *Physics of Fluids*, Vol. 27, No. 5, 052006 (2015).

Multiscale Poroelastic Modeling of Thermal Expansion of Concrete

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ABSTRACT

ABSTRACT The thermal expansion coefficient of concrete was reported to depend on the aggregate type, the volume fractions of the constituents, the age, and the internal relative humidity [1]. Concrete is a multiscale material consists of a cement paste matrix and aggregate inclusions. As for cement paste, the internal relative humidity increases with increasing temperature. This results in an unsymmetric bell-shaped dependence of the thermal expansion coefficient of cement paste on the internal relative humidity, varying between $8 \cdot 10^{-6} \text{ K}^{-1}$ to $22 \cdot 10^{-6} \text{ K}^{-1}$. The thermal expansion coefficient of the aggregate is typically smaller, ranging between $4 \cdot 10^{-6} \text{ K}^{-1}$ to $12 \cdot 10^{-6} \text{ K}^{-1}$, mainly depending on the mineral composition [1]. In this research, a multiscale poroelastic model for concrete is established, by resolving it down to nanoscopic hydration products. Measured changes of internal relative humidity serve as input, resulting in a variation of the effective pressure in both the gel and the capillary pores, as is the combined effect of the pore fluid pressure and the surface tension. The effective pore pressures are averaged as eigenstresses based on the proposed size distribution model of the pores [2,3]. Simultaneously, thermal eigenstresses are induced in the solid constituents, namely, solid hydrates, unhydrated clinkers, and aggregates, in case of a temperature change, linked to the macroscopic thermal expansion of the concrete with the multiscale model. The model is validated by comparing the predicted thermal expansion coefficients of cementitious materials with the experimental measurements. ACKNOWLEDGEMENTS Financial support by the Austrian Science Fund (FWF), provided within project P 281 31-N32 "Bridging the Gap by Means of Multiscale Structural Analyses", is gratefully acknowledged. The first author also gratefully acknowledges financial support by the China Scholarship Council. REFERENCES [1] J. H. Emanuel, J. L. Hulse, "Prediction of the thermal coefficient of expansion of concrete", Journal of the American Concrete Institute, 74(4), 149-155 (1997). [2] B. Pichler, C. Hellmich, "Estimation of influence tensors for eigenstressed multiphase elastic media with nonaligned inclusion phases of arbitrary ellipsoidal shape", Journal of Engineering Mechanics, 136(8), 1043-1053 (2010). [3] H. Wang, C. Hellmich, Y. Yuan, H. Mang, B. Pichler, "Does reversible water uptake/release by hydrates govern the thermal expansion of cement paste? – A scale transition analysis", Cement and Concrete Research, under revision.

A Simple Two-dimensional Mechanical Metamaterial with Negative Poisson's Ratio

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ABSTRACT

Abstract Metamaterials with negative Poisson's ratio, also named as auxetics, have attracted much effort towards exploring their applications as foldable devices in multiple engineering fields such as the medical and the aerospace fields, due to their counter-intuitive mechanical properties. In this study, a simple two-dimensional structure exhibiting auxetic behavior in both compression and tension is designed, which is different to the popular re-entrant or chiral designs. This is achieved by introducing peanut-shaped holes with different locations and rotational angles in linear elastic medium. Several auxetic configurations are fabricated by 3D printing technique and then studied through the computational and experimental methods to reveal their deformation mechanisms and characterize their compressive and tensile mechanical properties. It is found that the present modeling yields explicit mechanical properties including Poisson's ratios, strength and stiffness under tension and compression. Therefore, the methodology used by this study could be effectively employed to design two-dimensional auxetic matamaterials for various applications. References [1] T. Frenzel, M. Kadic, M. Wegener. Three-dimensional mechanical metamaterials with a twist. *Science* (2017)358, 1072–1074 [2] L. Yang, O. Harrysson, H. West, D. Cormier. Modeling of uniaxial compression in a 3D periodic re-entrant lattice structure. *J Mater Sci* (2013)48: 1413–1422 [3] X. Ren, J. Shen, A. Ghaedizadeh, H. Tian, Y.M. Xie. A simple auxetic tubular structure with tuneable mechanical properties. *Smart Mater Struct* (2016)25: 065012

A Three-dimensional Explicit Constitutive Model for High-precision Simulation of Concrete Structures

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ABSTRACT

Recently, a three-dimensional (3D) explicit constitutive model has been developed for numerical simulation of reinforced concrete (RC) and steel concrete (SC) structures. The proposed model is based on smeared crack model and fixed angle crack assumption. The decoupling of normal and shear stress after cracking is assumed for the concrete material to simulate the spatial cracking phenomenon of RC and SC structures. The uniaxial constitutive law is adopted from many existing literatures and shows good agreement with existing test data in terms of the tension stiffening, shear softening and compression softening of concrete material. The material model is implemented in ABAQUS software for both the implicit solver and explicit solver. The proposed model is calibrated and validated by a large number of existing tests in the literatures, including the panel tests, the shear wall test and the beam tests. The modeling scheme, material constitutive law, and material parameters are illustrated in detail. The results of the proposed FE model agree fairly well with existing test results in terms of the overall load–displacement curve, ultimate capacity, and failure pattern.

Data-augmented Multi-scale Modeling of Intracranial Pressure Dynamics

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ABSTRACT

Accurate intracranial pressure (ICP) monitoring is highly significant in a number of neurosurgical applications, and elevated ICP may lead to severe brain damage. The standard ways for clinical ICP monitoring are all invasive, which typically requires a hole drilled in the skull and transducer inserted into a ventricle [1]. This exposes the patient to infection and hemorrhage, and often requires a neurocritical care unit. Therefore, noninvasive estimation of ICP (nICP) is highly compelling for patient safety and broader access. Numerous past efforts on nICP attempt to identify ICP-related noninvasive signals or surrogates. These efforts while promising have not gained traction. To improve nICP prediction, we developed a data-augmented framework that combines a physical intracranial model and noninvasive signals using advanced data assimilation techniques. Conceptually, the proposed framework consists of three modules: (1) a forward model of the intracranial dynamics, (2) noninvasive measurement data, and (3) a data assimilation scheme. A multiscale cerebrovascular model [2] is used for simulating the forward intracranial dynamics. Noninvasive cerebral blood flow velocity (CBFV) measured by Transcranial Doppler Ultrasonography (TCD) is used for data assimilation. A regularizing iterative ensemble Kalman method is implemented to assimilate the TCD measured data into our physical model to improve predictive accuracy. For proof-of-concept, we first use synthetic TCD data to validate and examine the proposed framework. The synthetic observations are generated from the physical model with a set of specified model parameters as the "ground truth". Only CBFV at the left and right middle cerebral arteries (MCA) are observed and 10% random noise is added. By assimilating these synthetic data, the unobserved intracranial states (e.g., ICP, CBFV at non-measurable arteries) can be significantly better estimated. Preliminary application of this framework to clinical data where invasive ICP has been measured concurrently with TCD also demonstrates significant improvement of mean ICP prediction. By using both synthetic and real TCD measurements, we demonstrated that estimation of intracranial dynamics can be significantly improved by combining an imprecise model with imprecise and indirect noninvasive measurements. Future work includes gearing the hemodynamics-based physical model more toward ICP dynamics and potentially assimilating measurements that are more directly related to ICP than MCA flow velocity. References [1] X. Zhang, et al., *Physiol Meas* 38, R143 (2017). [2] J. Ryu, X. Hu, S. C. Shadden, *J Biomech Eng* 137, 101009 (2015).

Development of Maneuvering Control Module in CFD Solver naoe-FOAM-SJTU

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ABSTRACT

Maneuverability is one of the most concerned ship performance. So far, many studies have been done to predict maneuvering behavior using numerical methods, among which most are using the simplified model, either mathematical model or body force. Consequently, the detailed flow around ship hull, rotating propellers and moving rudders cannot be resolved during the maneuvering motion. In the present work, maneuvering control module is developed based on the CFD solver naoe-FOAM-SJTU, which has overset grid capability and a full 6 Degrees of Freedom (6DoF) motion module with a hierarchy of bodies. The implementation of the maneuvering control module is inherited from the motion module with a hierarchy of bodies, where moving components, such as propeller and rudder, are acted as the base of specific maneuvering controller. The control module adopts the feedback mechanism to deal with the motion of propellers and rudders. At present, three types of control module are achieved, i.e. heading controller, zigzag controller and turning circle controller. In addition, the open source toolbox waves2Foam is utilized to the present solver to simulate ship maneuver in waves. Based on the maneuvering control module, RANS computations are conducted to directly simulate free running ship maneuver with rotating propellers and moving rudders. The developed solver has been applied to various maneuvers, such as standard zigzag maneuver in both calm water and waves, turning circle maneuver in calm water and course keeping maneuver in various heading waves. During the simulation, the calculations start from the steady state of the self-propulsion calculation and the twin rudders are executed by a feedback control mechanism. The main parameters of ship maneuver, such as the overshoot angle, period, turning diameter and rudder deflection are obtained to compare with the available experiment data. Good agreement is achieved for both maneuvering parameters and ship motions. It shows that the present implementation of maneuvering control module is robust and reliable in simulating free running ship maneuver in both calm water and waves. Furthermore, the present approach can be easily extended to various control modules based on feedback control mechanism.

Phase Field Modeling of Ferroelectric Material with Isogeometric Analysis

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ABSTRACT

Isogeometric analysis (IGA) is a recently developed technology in computational mechanics. Its main idea is to use the same smooth and higher-order basis functions, e.g. non-uniform rational B-splines (NURBS), for the representation of both the geometry in CAD and the approximation of solution fields in analysis. Thus, the complex geometry of materials can be modeled exactly. As a consequence, geometric errors are eliminated. In addition, the high order continuities of the basis functions are ideally suitable for solving high order partial differential equations, like the equation of flexoelectric problems and Cahn-Hilliard equation, which require at least C^1 continuous approximations. These attributes permitted us to derive accurate, efficient, and geometrically flexible methods for the problems with higher-order derivatives. In this paper, a NURBS-based variational formulation for the phase field equations of ferroelectric materials is established. Several numerical examples are provided in this paper to confirm the accuracy of this method. After that, the polarization distributions inside the PbTiO_3 material are simulated with the help of IGA. Moreover, the polarization distribution inside a three-dimensional ferroelectric material with the consideration of flexoelectricity is obtained in this paper.

Single and Multi-Objective Aerodynamic Shape Optimizations by Means of Stackelberg Game Coupled with Adjoint Method

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ABSTRACT

Aerodynamic shape optimization in aeronautical engineering, by its nature, is multi-objective. In general, two approaches are mainly used for solving multi-objective optimization problems: (1) The weighted average optimization method. It aggregates all the objective functions with different weights to form a single function for optimization. Consequently, the design results strongly depend on the choice of reasonable weights. (2) The non-dominated optimization method based on evolutionary algorithms. The evolutionary process is very time consuming due to a large number of function calls. Therefore, this method is limited to solve problems with simple configurations and a small number of design variables. In this study, the Stackelberg game strategy is coupled with the continuous adjoint method to solve multi-objective aerodynamic shape optimization problems. In the game, two types of players (leader and follower) are involved, and each pair of players is responsible for the optimization of one objective function. During the game, players perform optimizations alternately using the continuous adjoint method until the leader cannot improve its objective function further. When the leader and the follower optimize the same objective function, a "virtual" multi-objective problem is formulated, and this game can also be used to solve single-objective optimization problems. Note that the success of the proposed method highly depends on the choice of a few critical parameters, including the maximal number of iterations for each player, the splitting scheme of design variables, and the assignment of objective functions and design variables to different players. Therefore, impacts of these parameters are firstly assessed by a simple optimization case while some useful inferences are produced for the choice of these parameters. For the RAE2822 airfoil and the ONERA M6 wing, single-objective and multi-objective aerodynamic optimizations are conducted to verify the usefulness of these inferences, and to validate the efficiency and effectiveness of the proposed optimization method with a large number of design variables. Moreover, it is found that when solving single-objective problems, the proposed method can provide better optimization results with less computational cost than the original continuous adjoint method. Keywords: Stackelberg game, Continuous adjoint method, Single-objective optimization, Multi-objective optimization, Aerodynamic shape optimization

The Stability Problems in SPH Numerical Wave Tank

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ABSTRACT

The numerical wave tank is one of the effective tools to study the wave and its effect on the floating structure. Compared with the traditional methodology of CFD to construct the tank, the Smoothed Particle Hydrodynamics (SPH) method is superior in dealing with problems concerning complex boundary and extremely large deformation. When traditional SPH method is used to simulate wave propagation in a wave tank? it is usually observed that the wave height attenuates and the wave length elongates along the direction of wave propagation, owing to the stability problems in SPH. Although the instability cannot be removed under any circumstances in traditional SPH, it can be improved in several aspects. At first, the effect of boundary condition would be discussed. Repulsive boundary condition, dynamic boundary condition, as well as, mirror particle boundary condition has been used in this 2D numerical wave tank. Secondly, as we all know, the kernel function plays an important role in the stability of pressure, which may be the main reason of the problem. At the same time, the quality of wave varies with different smooth length in the kernel functions. Hence, the selection of kernel function and the smooth length would be talked in the paper. At last, some improvement of SPH methods, such as δ -SPH and GSPH, and other numerical processing techniques, would be taken into this wave tank to improve the stability of the numerical tank. Their adaptive in wave generation and propagation is shown in the simulations. By the research of these three aspects, a stable SPH numerical wave tank is established with little attenuation. Reference [1]Antuono M, Colagrossi A, Marrone S, et al. Propagation of gravity waves through an SPH scheme with numerical diffusive terms[J]. Computer Physics Communications, 2011, 182(4):866-877. [2]Kunal Puri, Prabhu Ramachandran. Approximate Riemann solvers for the Godunov SPH (GSPH)[J]. Journal of Computational Physics, 2014, 270(8):432-458. [3] Zhang J Z, Zheng J, Kai-Ping Y U, et al. A RESEARCH ON THE TENSILE INSTABILITY OF SPH IN FLUID DYNAMICS[J]. Engineering Mechanics, 2010, 27(2):65-72.

A Wavelet Method on the Solution of Nonlinear Problems in Computational Material Sciences

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ABSTRACT

A high-order wavelet method is developed for general nonlinear boundary value problems in mechanics. This method is established based on Coiflet approximation of multiple integrals of interval bounded functions combined with an accurate and adjustable boundary extension technique. The convergence order of this approximation has been proven to be N as long as the Coiflet with $N-1$ vanishing moment is adopted, which can be any positive even integers. Error analysis has proven that the proposed method is order N , and condition numbers of relevant matrices are almost independent of the number of collocation points. Examples of a wide range of strong nonlinear problems in engineering, especially in mechanics, including the extremely large deflection bending of plates and shells with complex shapes, demonstrate that accuracy of the proposed method is even greater than N , and most interestingly, such accuracy is independent of the order of the differential equation of the problem to be solved. Comparison to existing numerical methods further justifies the accuracy and efficiency of the proposed method.

Hybridizing Neural Network and Hand-crafted Critical State Plasticity Model for Forward Prediction of Geomaterials in a Directed Graph

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ABSTRACT

This work presents a novel component-based approach on the development of constitutive models for materials having complex path-dependent mechanical properties. Critical state plasticity models for capturing the complex cyclic response of sands have been proposed, yet lack the prediction accuracy against experiments. To extend the capability of the existing models, we propose the introduction of machine learning on experimental data into the conventional plasticity formulations. The directed graphs of the constitutive models are constructed, with the nodes representing the physical quantities (stress, strain, porosity, fabric tensor, etc.) and the edges representing the universal principles, definitions or constitutive equations relating these quantities. The discrepancy between the different constitutive models lies in the configuration of the directed graphs. The fully mathematical plasticity model involves yield surfaces, plasticity potentials, and evolution equation of internal variables. The fully data-driven constitutive model relates the stress to strain directly via the neurons in the artificial neural networks conserving material frame indifference. The development of hybrid data-driven plasticity model consists of selective replacement of mathematical formulation by machine learning. The choices of data-driven nodes and edges in the directed graph result in different configurations, hence lead to different hybrid models. We present a group of model designs with various degree of hybridization and compare them against experimental data on cyclic responses of sands. Their accuracy and computational efficiency are compared within our proposed model evaluation framework. This work offers the community a novel graph-based systematic approach on developing and assessment of hybrid data-driven constitutive models.

On the Use of Advanced Material Point Methods for Problems Involving Large Rotational Deformation

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ABSTRACT

The Material Point Method (MPM) is a quasi Eulerian-Lagrangian approach to solve solid mechanics problems involving large deformations. The standard MPM discretises the physical domain using material points which are advected through a standard finite element background mesh. The method of mapping state variables back and forth between the material points and background mesh nodes in the MPM significantly influences the results. In the standard MPM (sMPM), a material point only influences its parent element (i.e. the background element in which it is located), which can cause spurious stress oscillations when material points cross between elements. The instability is due to the sudden transfer of stiffness between elements. It can also result in some elements having very little stiffness or some internal elements losing all stiffness. Therefore, several extensions to the sMPM have been proposed, each of which replaces the material point with a deformable particle domain. The most notable of these extensions are the Generalised Interpolation Material Point (GIMP), the Convected Particle Domain Interpolation (CPDI1) and Second-order CPDI (CPDI2) methods. In this paper, the sMPM, CPDI1 and CPDI2 approaches are unified for geometrically non-linear elasto-plastic problems using an implicit solver and their performance investigated for large rotational problems. This type of deformation is common in applications in the area of soil mechanics, for example the vane shear test and, specifically of interest here, the installation of screw piles. Screw piles are currently used as an onshore foundation solution and research being undertaken at Durham, Dundee and Southampton universities is exploring their use in the area of offshore renewables. The numerical modelling using the MPM aims to predict the installation torque and vertical force as well as understanding the "state" of the soil around the screw pile which is critical in understanding the long term performance of the foundation. In the analysis, the pile is assumed to be a rigid body and no-slip boundary condition is used at the pile-soil interface. The boundary condition is imposed using the moving mesh concept within an unstructured mesh fixed to the pile. It will be shown that the CPDI2 approach produces erroneous torque due to particle domain distortion, while the CPDI1 approach and sMPM predict physically realistic mechanical responses.

Applications of Enhanced Sampling Methods in Protein-ligand Binding Free Energy Calculations

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ABSTRACT

Accurate and reliable calculation of protein-ligand binding free energy is of central importance in computational biophysics and computer aided drug design. While alchemical free energy perturbation (FEP) methods provide an in-principle most rigorous approach for protein-ligand binding free energy calculations and are expected to yield the most accurate predictions, the accuracy of free energy calculations had been hindered by inadequate sampling of protein-ligand conformational space, blocking their applications in drug discovery projects. In this presentation, I am going to talk about the enhanced sampling method REST2 (Replica Exchange with Solute Tempering), designed to efficiently sample the complex potential energy surfaces of biological molecules. In particular, I am going to focus on the applications of REST2 on free energy calculations (through FEP/REST), and present the large-scale testing of FEP/REST on protein-ligand binding free energy calculations. We demonstrate that the combination of FEP/REST and the accurate force field OPLS3 achieves an unprecedented level of accuracy in protein-ligand binding free energy calculations across a broad range of target classes and ligands and a wide variety of chemical perturbations, and positions free energy calculations to play a guiding role in small molecule drug discovery.

Wave Propagations in Linear Elastic Peridynamic Media

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ABSTRACT

The elastic waves in peridynamic media are different from those in the classical local media. The dispersive characteristics of waves in bond-based peridynamics have been studied in the literature, but the general properties of the waves in the state-based peridynamic media are less investigated. In particular, the integral forms raise great obstacles in mathematics to analytically investigating the properties of the state-based peridynamic theory. In this work, we focus on the dispersive characteristics of waves in state-based peridynamics. We examine in detail the dispersion relations, group velocity, phase velocity for different constitutive relations of the peridynamic media, and for different Poisson's ratios. We find that the wave velocity in peridynamic media with negative Poisson's ratios may be larger or less than that in the corresponding local media. These results have particular implications in analysing wave propagations in heterogeneous media.

VCUT Level Set: A Level Set Method with Variable Cutting Functions for Topology Optimization of Multiscale Structures

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ABSTRACT

In this paper, we introduce a novel level set method with variable cutting, called VCUT Level Set, for designing topologically variable cellular structures through geometric modeling and structural optimization. In the conventional level set method for implicit representation of a structure as usually applied in structural topology optimization, the height level of the level set function is set at a constant value (i.e., zero). The basic idea of the VCUT level set approach is to replace the constant-valued cutting height (i.e., zero) with a variable-valued cutting function which is defined and characterized by a set of parameters, such as a piece-wise linear function or a parametric (nonlinear) function. These parameters of the variable cutting function are incorporated as variables as well in the numerical process of optimization. The VCUT level set method provides a greater capability and flexibility for optimizing not only solid macro-structures, but also cellular structures at micro- and meso- scales concurrently. In a demonstration of the VCUT level set method, we first define a global mesh over the design domain of the structure. The set of cutting heights are defined on the mesh nodes and they in turn interpolate a cutting function (linear or higher order) within each mesh element, to be applied locally to the level set function within the element. Since the cutting height is applied by the shared nodes and is interpolated within the mesh element, full geometric continuity in the level set representation is guaranteed at the face between two neighboring elements. In this paper, we apply the VCUT level set method for multiscale design of structures with spatially-varying mesoscale cells. The topology optimization seeks both the best cell geometry and the optimal distribution of graded cells. Numerical examples demonstrate the capabilities of the proposed VCUT level set method for optimizing multiscale structures with unprecedented macroscale topological features and mesoscale cellular distributions with smooth spatial gradient.

Strengthening Mechanisms in Surface Nano-crystallized Metals

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ABSTRACT

Surface nano-crystallized (SNC) metals have great potential applications due to its good balance of strength and ductility. However, the strengthening and toughening mechanisms are still elusive because the grain size spans over four orders of magnitude in the gradient structure, suggesting that the corresponding constitutive behaviors vary obviously across several length scales. After analyzing the evolution of microstructure and mechanical characteristic of SNC copper at various scales, three different kinds of constitutive behaviors associated with the coarse grain (CG) layer, the transitional grain (TG) layer and the gradient nano-grain (GNG) layer are identified. Therefore, the evolution equations of dislocation density of these layers are needed to be established. Subsequently, we develop a general approach within the framework of dislocation mechanism based crystal plasticity to characterize the corresponding constitutive behaviors. Then, the strengthening mechanisms of SNC metals are analyzed within the framework. It is shown that the predictions based on the framework are in good agreement with the experimental results and the plastic strain gradient produce the non-local strengthening effect which is similar to the mechanism responsible for the strengthening of thin film passivated on one or both sides. The proposed general framework is capable of optimizing the mechanical properties and investigating the subsequent failure process in SNC materials. Keywords: Surface nano-crystallized metal, General constitutive model, Dislocation density evolution, Dislocation-based crystal plasticity, Non-local effect

Reliability Analysis of a MASH TL-3 Concrete Median Barrier Using Metalmodels and FORM

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ABSTRACT

Concrete median barriers are rigid barriers that are widely used on U.S. freeways. In this research work, reliability analyses of concrete median barriers under vehicle crashes were studied. The concrete barriers were under vehicular crashes according to the Manual for Assessing Safety Hardware (MASH) test level 3 (TL-3) requirements. In the proposed approach, a metamodeling method based on augmented radial basis function (RBF) was integrated with a First-Order Reliability Method (FORM). The random variables included impact parameters such as the vehicle weight and impact angle. Various crash responses were evaluated using computational methods and nonlinear transient finite element (FE) analyses. To reduce the computational effort due to the expensive numerical simulations, an approximation technique was applied and the augmented RBF metamodels were constructed to express the performance functions. One of the compactly supported RBFs augmented with linear polynomials was adopted, which was identified to be an accurate RBF from the authors' previous work. An alternate FORM was implemented once explicit expressions of the performance functions became available. This reliability analysis approach was tested for various mathematical and engineering examples. In the application to concrete barriers, different vehicular responses and occupant responses including those defined in the current crash standard were adopted and their limit values were selected. Reliability analyses were performed using the new approach and the failure probabilities and reliability indices were obtained. The reliability analysis results provided useful information for the assessment of concrete barriers. This proposed approach is useful for impact problems requiring expensive simulations and reliability analyses of these problems become more important for design optimization and decision making.

Contribution of Elastin and Collagen to Inter-Lamellar Bonding in the Arterial Wall

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ABSTRACT

Arterial wall delamination begins with a tear cutting in the intima, which allows blood flow to enter the newly created lumen and split the media. To date, little is known about the distinct role of elastin and collagen plays in the initiation and propagation of aortic wall delamination. Elastin and collagen forms the primary load bearing extracellular matrix (ECM) components in the arterial wall. In fact, 27% of elastin was found to protrude obliquely from lamellar surfaces and terminate in inter-lamellar space, and 2% of elastin was found in the form of radial elastin struts that provides direct radial connection between adjacent lamellae [1]. This study aims to understand the contribution of elastin and collagen fibers to inter-lamellar bonding in the arterial wall. Peeling tests were performed on porcine thoracic aorta and purified elastin network. The peeling force/width in aortic media is about five times of that in elastin network, indicating the important role of inter-lamellar collagen in maintaining arterial wall integrity. In-situ multi-photon images revealed the presence of both inter-lamellar elastin and collagen fibers at the separation site between lamellar layers. A finite element model of peeling tests was created based on cohesive theories of fracture [2]. A hyperelastic and anisotropic constitutive law was used to model the tissue behavior [3]. Simulation results were fitted to experimental load-displacement curves to estimate the inter-lamellar bonding stiffness, stresses at damage initiation and fracture displacement in the cohesive zone for aortic media and elastin network. Resistance to inter-lamellar debonding was found to be the main contributor to the differences in peeling forces between aortic media and elastin. For cohesive interfaces following a bilinear traction-separation damage law, much higher bonding stiffness and damage initiation stresses were obtained in aortic media than in elastin network. Removal of collagen reduced inter-lamellar fiber density, which leads to the decreased bonding in elastin network. To consider the distinct role of elastin and collagen plays in the initiation and propagation of aortic wall delamination, a more realistic multiscale traction-separation relation for the cohesive zone was developed to include the structural and mechanical contributions of elastin and collagen fibers. [1] O'Connell M.K et al., *Matrix Biol*, 27:171–181, 2008. [2] Hillerborg A et al., *Cem Concr Res*, 6:773-782, 1976. [3] Holzapfel G.A et al., *J Elast*, 61:1-48, 2000.

Experimental Study on Mechanical Properties of Human Facial Skin in Vivo

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ABSTRACT

Characterising the mechanical behavior of human skin is of great importance for a number of applications including surgery, animation, dermatology and biomechanics. The human skin, which covers almost entirely the human body, is a complex multi-layer material, composed of epidermis, dermis and hypodermis. With nonlinear behavior, anisotropy, viscosity and preconditioning effects, it is a challenging endeavour to study mechanical properties of human skin. Furthermore, it depends on many factors, such as ageing, environment and in vivo or in vitro. In this study, the effect of different thickness of skin tissue and probe size have been investigated. To consider the bone, we propose a two-layer theoretical model. A novel loading device applied to the facial skin is developed. It can realize a precise three-dimensional (3D) translation, and the contact force can be measured with a loading cell. In order to ensure an indentation normal to the surface, we use a CCD camera combined with a transparent probe is employed to measure the contact area during loading and to analyze its contact state. The thickness of facial skin tissue are measured by the head CT photographs of subjects. We focus on the measurement of the mechanical behavior of facial skin tissue in vivo, combining the experimental test with the finite element method to study the mechanical constitutive mechanism of the facial soft tissue.

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Study on Formation Mechanism of Hydraulic Fracturing Network of Layered Shale

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ABSTRACT

Shale is a typical heterogeneous and anisotropic material whose properties are characterized primarily by locally oriented anisotropic clay minerals and naturally formed bedding planes. The nature of the bedding planes will greatly affect the hydraulic fracturing of the shale to form a large-scale stimulated reservoir volume (SRV). In this paper, the debonding behavior of bedding planes in the process of hydraulic fracture (HF) propagation is studied. Two dimensionless parameters are proposed to characterize the difficulties of tensile and shear debonding of the bedding planes. By analyzing the two dimensionless parameters, it can be found that the SRV is mainly caused by the shear failure of bedding planes in the actual hydraulic fracturing treatment. The larger the shear strength of the rock or the smaller the net fluid pressure, the smaller the SRV and the optimal perforation cluster spacing. Two dimensionless parameters (stimulating volume ratio and stimulating efficiency) are proposed to evaluate the stimulating effect. According to the theory of debonding in this paper, it is possible to guide the treatment of hydraulic fracturing, predict the SRV, optimize the spacing of perforation clusters, and improve the production of shale gas.

Meso-scale Nonequilibrium Features in a Gas-Fluidized Bed

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ABSTRACT

To understand the meso-scale, far-from-equilibrium behavior in fluidization [1], we investigate, both numerically and experimentally, the nonequilibrium features in a pseudo 2D bubbling fluidized bed. In experiment, velocities of individual particles are measured by using a particle tracking velocimetry (PTV) method, and void fractions are obtained with Voronoi tessellation. A bimodal shape of probability density function (PDF) for particle vertical velocity is found in not only time-averaged but also time-varying statistics, which is caused by the transition between the dense and dilute phases and breaks the local-equilibrium assumption in continuum modeling of fluidized beds [1]. The results of time-varying radial distribution function and voidage distribution also confirm this finding. Moreover, analysis of voidage, velocity of particle, granular temperature and turbulent kinetic energy of particles shows that there is no scale-independent plateau over the interface, and it seems hard to find a scale-independent plateau to separate the micro- and meso-scales of fluidized beds, which require sub-grid meso-scale modeling for continuum or coarse-graining methods of gas-fluidized systems [2]. In numerical simulation, dense discrete particle method is used with the energy minimization multi-scale (EMMS) drag. Simulation results generally agree with the experiment. References [1] W. Wang, Y. Chen, Mesoscale modeling: Beyond local equilibrium assumption for multiphase flow, *Adv. Chem. Eng.* 47(2015) 193–277. [2] Y. Tian, J. Geng, W. Wang, Structure-dependent analysis of energy dissipation in gas-solid flows: Beyond nonequilibrium thermodynamics, *Chem. Eng. Sci.* 171 (2017) 271–281.

Probing the Mechanical Interactions of Cell Nuclear Pore Complex with Nanoparticles

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ABSTRACT

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.

Modeling the Crystal Growth of Semi-crystalline Polymers by a Phenomenological Phase-field Method

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ABSTRACT

Crystal growth of either polymers or metals commonly shows distinct anisotropic behaviors related to the anisotropy of interfacial free energy. Most of the phase-field models developed for solidification use a simple anisotropic function, which makes the interfacial free energy (the gradient term) depend on direction, to describe the anisotropic crystal growth [1]. The frequently used cubic anisotropic function in 3D [2], which has equal strength of anisotropy in the six main directions, only can be used to simulate the equiaxed dendritic growth pattern. For semi-crystalline polymers, because the alignment of molecular chains in some directions is often promoted or confined [3], the anisotropic crystal growth is seldom equiaxed. Therefore, it is necessary to derive new anisotropic functions special for semi-crystalline polymers. In this study, we have established a 3D phase-field model for investigating the crystal growth of semi-crystalline polymers. The model can be regarded as a generalization of the 2D phase-field model we ever presented. It couples a nonconserved crystal order parameter with a temperature field generated by latent heat of crystallization, and obtains its model parameters from the real material parameters. Unlike the models of metals and small molecular compounds, the current model considers the partially crystallization property of semi-crystalline polymers. Moreover, due to the long-chain molecular structure, polymer crystallizations usually exhibit complex anisotropy and have polymorphous nature. To account for the various anisotropy of interfacial energy in 3D, three anisotropic functions describing the anisotropic interfacial growth patterns are deduced phenomenologically based on a number of existing experimental facts. Simulation results have preliminary demonstrated the good performance of our phase-field model in reproducing the complex and diverse morphology of semi-crystalline polymers in 3D. Several kinds of crystal patterns, which have been observed in experiments, can be reproduced. [1] Xu, H.J.; Matkar, R.; Kyu, T. Phase-field modeling on morphological landscape of isotactic polystyrene single crystals. *Phys. Rev. E* 2005, 72, 011804. [2] Karma, A.; Rappel, W.J. Quantitative phase-field modeling of dendritic growth in two and three dimensions. *Phys. Rev. E* 1998, 57, 4323–4349. [3] Wang, H.P.; Jong, K.K.; et al. Confined Crystallization of Polyethylene Oxide in Nanolayer Assemblies. *Science* 2009, 323, 757–760.

Explicit Multi-material Topology Optimization of Freely Vibrating Continuum Structures Using Moving Morphable Bars

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ABSTRACT

It is accepted that the existing literature on dynamic optimization problem is all carried out in an implicit way, which involves a large number of design variables. More recently, a new class of optimization methods based on discrete geometric components has been proposed with the aim of doing topology optimization in an explicit and flexible way. In this paper, an explicit multi-material topology optimization method is developed for freely vibrating continuum structures, where the geometric parameters used to describe the size, shape and location of the moving bars are considered as design variables of the optimization problem. The moving bars corresponding to different material phases are mapped into two density fields on a fixed grid using a smoothed Heaviside function, which can not only avoid remeshing the grids but also enable us to use gradient-based algorithms to solve optimization problems. The explicit model of multi-material topology optimization using moving morphable bars and its sensitivity analysis is detailed for two different optimization problems, including maximization of the n -th eigenfrequency and Maximization of eigenfrequency gap. Numerical examples demonstrate the present formulation provides an effective means for multi-material topology optimization of freely vibrating continuum structures.

Adaptive Solution Transfer Between Non-matching Meshes for Coupling Climate Models

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ABSTRACT

Solution transfer is a critical component in global climate modeling, which requires coupling an atmospheric model with the ocean, land, sea-ice models, etc. These models may utilize different numerical discretization methods, and hence the interface meshes between them may be non-matching. Some of these models increasingly utilize high-order numerical methods and higher-resolutions meshes. It is necessary to develop more robust and efficient solution transfer methods, which must support high-order methods at various grid resolution. The commonly used solution-transfer methods are either pointwise-based (such as interpolation or moving least squares) or integral-based (such as the common-refinement or super-mesh based methods). The former is efficient but not conservative, while the latter is conservative but typically requires computing the intersections of the cells, which is geometrically complicated and computationally expensive. In this work, we propose an adaptive solution transfer method, which can achieve approximate local conservation in a weighted sense, without requiring the computation of intersections of the cells. To this end, our method uses the generalized Lagrange polynomial (GLP) basis functions in a Petrov-Galerkin formulation, in which the test functions are adapted to accommodate large gradients and potential discontinuities in the solution. Our method supports transferring node-based, cell-centered, or cell-averaged values in finite elements, finite volume, or spectral element methods. It can achieve high-order accuracy with excellent long-term stability. We demonstrate the approach using exchanges of heat and mass in a coupled atmosphere-ocean model.

Action Feedback Control of Elastic Wave Metamaterials

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ABSTRACT

There are a large number of investigations about elastic waves in periodic structures which are called as phononic crystals or elastic wave metamaterials. In this kind of systems, we can find the stop band in which acoustic and elastic waves cannot propagate. Based on this characteristic, these structures can be applied to noise and vibration isolation, elastic wave filters, etc. And a lot of investigations are reported on how to tuning methods of stop bands in elastic wave materials. Although there have been many methods applied to control the stop bands, they are mainly focused on the passive ones which are not easily changed according to the external situations. But we know that the automatic control system combines the merits of both electrical and mechanical devices. Then we can change our attention on the active control action with the automatic system. On the other hand, most of the previous investigations on elastic wave metamaterials are about the linear case, only a few studies have been reported on nonlinear elastic waves. But nonlinear elastic waves can show quite different characteristics from linear ones. In this work, the influence of active feedback control on nonlinear elastic wave metamaterials is discussed. From the results, we can conclude that the active control method can change both the location and width of stop bands, which are suitable to practical engineering. Acknowledgements: The presented work is supported by the National Natural Science Foundation of China under Grant Nos. 11772039 and 11532001.

A High-fidelity Computational Model for AM Models with Manufacturing Errors

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ABSTRACT

Additive manufacturing (AM), with material being added together layer by layer, can be used to produce objects of almost any shape or geometry. However, AM techniques cannot accurately build parts with large overhangs, especially for the large features close to horizontal, hanging over void. The overhangs will make the manufactured model deviate from the design model, which may cause the performance of the manufactured model cannot satisfy the design requirements. In this work, we will propose a new finite element (FE) model that includes the manufactured errors by mimicking the AM layer by layer construction process. In such FE model, an overhang coefficient is introduced to each FE, which is defined by the support elements in the lower layer. By mimicking the AM process from the bottom layer to the top layer, all the FE properties are updated based on their overhang coefficients, which makes the computational model is able to accurately predict the manufactured model with manufacturing errors. The proposed model can be used to predict the performance of the AM objects in the design stage, which will help the designers to improve their design by the simulation results.

Vortical Structure Development in a Riblet Controlled Boundary Layer Transition

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ABSTRACT

The drag reduction mechanism of riblets with appropriate configuration is still unclear. In the present study, direct numerical simulations of flat plate and riblet controlled boundary layer transition are performed with Reynold number 1000 based on the inflow displacement thickness. It is found that the scalloped riblets investigated in this study induce streamwise vortices near the riblet tips which persist even after the flow become fully turbulence. In addition, a similar situation that the skin friction coefficient is highly correlated to the vortical structures in the log layer is found in both cases with and without riblet control, which justifies the need to study vortical structure development. The width and height of the scalloped riblet pose a great influence on the drag reduction performance. It is reported that riblets with width of wall unit 25-30 is optimised for drag reduction [1]. For the present study, the width of the scalloped riblet is 1.375 times inflow displacement thickness, which is in the range of 25-30 wall units. However, even though the averaged drag per unit area is substantially reduced around 20 percent, the total drag is not decreased at all because of the increase of we surface area. In this sense, a second case with same riblet shape, width and height, but with longer valley region is investigated. The results for this second case is still pending. The influence of riblets on the vortical structures will also be studied for the early transition stage. Klumpp et al. investigated how the same shape riblets advance or delay the boundary layer transition. In addition to their research, further detailed flow vortical structures will be given and their relationship to drag will also be investigated. [1] H. Choi, P. Moin and J. Kim, Direct numerical simulation of turbulent flow over riblets, *Journal of Fluid Mechanisms*, 1993, 255: 503-539. [2] S. Klumpp, M. Meinke, and W. Schroder, Numerical simulation of riblet controlled spatial transition in a zero-pressure-gradient boundary layer, *Flow Turbulence & Combustion*, 2010, 85, 57-71.

Steklov Geometry Processing: An Extrinsic Approach to Spectral Shape Analysis

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ABSTRACT

We propose Steklov geometry processing, an extrinsic approach to spectral geometry processing and shape analysis. Intrinsic approaches, usually based on the Laplace--Beltrami operator, restrict consideration to quantities that can be measured without leaving the surface, and thus cannot distinguish shapes that deform isometrically. While extrinsic approaches hope to completely capture and characterize a shape including its spatial embedding, many previous extrinsic methods lack theoretical justification or require meshing of the volume enclosed by a surface. Instead, we propose a systematic surface-based approach to spectral analysis via Steklov eigenvalue problem, which involves computing the spectrum of the Dirichlet-to-Neumann operator of a surface bounding a volume. The Dirichlet-to-Neumann operator is the linear map from the boundary Dirichlet data of a Laplace equation to its corresponding Neumann data. A remarkable property of this operator is that it encodes the extrinsic and volumetric geometry up to rigid motion. For example, a recent result due to Polterovich and Sher [2015] shows the Steklov spectrum encodes extrinsic quantities including mean curvature. We use the boundary element method (BEM) to discretize the operator, accelerated by hierarchical numerical schemes and preconditioning; this pipeline allows us to solve eigenvalue and linear problems on large-scale meshes despite the density of the Dirichlet-to-Neumann matrix. Our experiments verify that the Steklov eigenfunctions are volumetric-shape-aware and that they encode the extrinsic features missed by intrinsic algorithms. We further demonstrate that our operators naturally fit into existing frameworks for geometry processing, making a shift from intrinsic to extrinsic geometry as simple as substituting the Laplace--Beltrami operator with the Dirichlet-to-Neumann operator. As a result, a large range of applications, including shape exploration, comparison, segmentation, correspondence, geometry descriptor computation, and spectral distance computation can benefit immediately from our operator, without the need of a volumetric discretization. Reference: [Polterovich and Sher 2015] Iosif Polterovich and David A Sher. Heat invariants of the Steklov problem. *The Journal of Geometric Analysis* 25, 2 (2015), 924–950. [Wang et al. 2017] Yu Wang, Mirela Ben-Chen, Iosif Polterovich, and Justin Solomon. Steklov Geometry Processing: An Extrinsic Approach to Spectral Shape Analysis. arXiv:1707.07070. Under review.

Experimental and Numerical Study of Surface Characteristics of Ti-6Al-4V Alloy in High Speed Cutting Based on SHPB System

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ABSTRACT

Abstract: This paper investigated the surface characteristics of Ti-6Al-4V in high speed cutting based on split Hopkinson pressure bar (SHPB) system with both experimental and numerical methods. The high-speed cutting of Ti-6Al-4V titanium alloy was simulated by three-dimensional finite element method to study the effects of cutting speed and cutting depth on cutting force and residual stress. Based on the simulation results, the high-speed cutting experiment based on SHPB was carried out. The cutting force was measured by strain gauge, the residual stress of the machined surface were measured by X-ray diffraction and the roughness of the machined surface were measured by needle scanning. The results show that with the experimental cutting speed (4.5-9.5m/s) and the cutting depth (0.1-0.6mm), the cutting forces, surface roughness and residual stress in the direction of the cutting speed decrease with the increasing cutting speed. As cutting depth increases, cutting forces and surface roughness increase. Therefore, better surface quality could be got by choosing a small cut depth and large cutting speed. By comparing the experimental results of cutting force and surface residual stress with numerical results, it is found that the two have good consistency. Keywords: High speed cutting; Finite element simulation; Surface characteristics; Hopkinson pressure bar; Ti-6Al-4V Alloys References [1] Gao C-Y, Zhang L-C, Liu P-H. The role of material model in the finite element simulation of high-speed machining of Ti6Al4V[J]. Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, 2016, 230(17): 2959-2967. [2] Larbi S, Djebali S, Bilek A. Study of High Speed Machining by Using Split Hopkinson Pressure Bar[J]. Procedia Engineering, 2015, 114: 314-321.

A Novel Reliability Analysis Technique Based on Adaptive Kriging and Error Estimation

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ABSTRACT

As the complexity of numerical models, such as those based on FEM, increases and larger number of random variables are incorporated to enhance model completeness and predictability, the analysis of reliability of systems has become significantly more challenging. This is due to significant increase in the required number of calls to performance functions to achieve acceptable accuracy and increase in the computational time for each simulation. These challenges have motivated large efforts for development of reliability analysis algorithms that can substantially reduce the number of calls to performance functions, while maintaining high accuracy in reliability estimates. Surrogate model based approaches such as Support Vector Regression (SVR), Polynomial Chaos Expansion (PCE) and Kriging provide powerful tools for such reliability problems. Among these surrogate models, Kriging-based approaches can leverage statistical information via active learning to search for next best training points for model refinement. Well-known algorithms such as EGRA and AK-MCS leverage this property of Kriging to yield accurate estimates of failure probabilities. However, these algorithms lack the ability to determine error in their estimates of failure probability. Furthermore, the stopping criteria for the active learning process in these techniques are too strict, which can potentially lead to 'overfitting' phenomenon. To address the above limitations, the present paper introduces a new reliability analysis algorithm called Generalized Error Rate based Adaptive Kriging (GERAK). The structure of this algorithm is similar to AK-MCS. However, central limit theorem and its lemma De Moivre - Laplace theorem are employed to determine probabilistic properties of the number of realizations where the surrogate model yields wrong estimate for the sign of the limit state function. This feature is then used to reliably estimate an upper bound for error in failure probability estimates and subsequently as stopping criterion for refining the surrogate model. This along with the use of Maximum Uncertainty Function (MUF) as learning function that seeks for points with high uncertainty and probability density have led to very fast convergence of GERAK to true probability of failure. Several analytical examples are investigated in this study to showcase the significant advancements offered by GERAK compared to AK-MCS and other well-known methods.

Influence of Bubbles Growth and Detachment on a Catalytic Tubular Micromotor

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ABSTRACT

Self-propelled micromotors that can convert environmental energy into mechanical movement are ubiquitous in our bodies. Particularly, the bubble-propelled tubular micromotors play an irreplaceable role in biomedicine and other fields. The performance of bubbles inside the catalytic micromotor should be clearly studied to meet the challenges in these widespread applications. Accumulated experiments have already revealed that the motion and lifetime of bubble-propelled tubular micromotors can be deeply influenced by bubble size and generation frequency. A mechanical model considering the bubble growth and detachment inside the tubular micromotor has been proposed. The effect of bubble size on locomotion of bubble-propelled tubular micromotors has been studied. Numerical investigations of the motility-related parameters, such as bubble size and generation frequency, the average velocity and track lines of the micromotor, are proved to be dependent of the geometry of the micromotor, roughness of the inner wall of the tubular micromotor and concentration of solution in the surrounding cues.

A Spectral-Element/Fourier Smoothed Profile Method for Large-Eddy Simulations of Industrial-Complexity Wake Flows

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ABSTRACT

An accurate, fast and robust spectral-element/Fourier smoothed profile method (SEFSPM) for turbulent flow past 3D complex-geometry moving bluff-bodies is developed and analyzed in this paper. Based on the concept of momentum thickness, a new formula for determining an interface thickness parameter is proposed. In order to overcome the numerical instability at high Reynolds number, the so-called Entropy Viscosity Method (EVM) is developed. To overcome resolution constraints pertaining to moving immersed bodies, the Coordinate Transformation Method (Mapping method) is incorporated in the current implementation. Moreover, a hybrid spectral element method using mixed triangular and quadrilateral elements is employed in conjunction with Fourier discretization along the third direction to efficiently represent body of revolution or long-aspect ratio bluff-body like risers and cables. The combination of the above coupling method are validated by prototype flows including flow past a stationary sphere at Reynolds number in the range [200,1,000], turbulent flow past a stationary and moving cylinder at Reynolds number in the range [80,10,000], as well as turbulent flow past a flexible dual-step cylinder at $Re_D=2000$. Finally, the application to predict the response of a self-excited flexible riser consisting of buoyancy-modules with aspect ratio over 50 at $Re_D=1000$ demonstrates that SEFSPM is a promising choice for industrial-complexity turbulent flows.

A Coupled Gradient-Based Shape and Topology Optimization Method

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ABSTRACT

Abstract: Topology optimization is a widely-used technique for finding the most favorable, internal structural lay-out with a minimal weight under the specific loading and boundary conditions applied[1,2]. Accordingly, within a finite element setting this technique searches for the optimal relative density of a fixed, discretized spatial domain representing the actual structure. To enable more diversity within the design domain and to enlarge the search space of optimal structural configurations, in the present work a coupled method for topology optimization and shape optimization is proposed. The method incorporates the shape design variables into a SIMP (Simplified Isotropic Material with Penalization) topology optimization formulation, whereby the shape and topology optimization steps are performed in a sequential manner. The computational efficiency of the method is warranted by using Non-Uniform Rational B-Splines (NURBS) for describing the outer shape of the design domain, and by combining gradient-based optimization solvers with analytically derived shape and topology sensitivities. The coupled method has been implemented in a finite element framework to analyze 2D, 2.5D, and 3D structural design problems. The results of representative case studies clearly show that the features of the design domain can have a large influence on the final topology calculated. Additionally, the optimization sequence in the coupled method may affect the path followed within the design space; however, this typically only has a minor effect on the final computational result. [1] Bendsøe, M.P., Sigmund, O. (2004). Topology optimization by distribution of isotropic Material. In Topology Optimization (pp. 1-69). Springer, Berlin, Heidelberg. [2] Sigmund, O., Maute, K. (2013). Topology optimization approaches. Structural and Multidisciplinary Optimization, 48(6), 1031-1055. Keywords: Structural design, Shape optimization, Topology optimization, Coupled model.

Numerical Modeling of Oligocrystalline Shape Memory Alloys

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ABSTRACT

Shape memory alloys (SMAs) are a class of metal alloys that can recover their original shapes when heated above a certain temperature. Unique features including the superelasticity and shape memory effect have made shape memory alloys attractive materials for a variety of fields ranging from bioengineering to aerospace engineering. In polycrystalline forms, the desirable properties of SMAs have been tremendously compromised by the brittleness problem due to severe premature intergranular fractures around grain boundaries and triple junctions. To overcome the problem of detrimental intergranular fracture, Chen et al. (2009) designed Cu-based SMAs in fine wire forms with bamboo-shaped oligocrystal microstructure. Experiments show that, by carefully designing the microstructure of oligocrystalline SMAs (oSMAs), mechanical properties approaching those of a single crystal can be achieved without being limited by various constraints involved in single crystal processing. It is, thus, of great importance to investigate how the microstructure and grain boundary characters affect the phase transformation and transformation-induced fracture of oSMAs. To study the impact of grain constraints on the ductility limits and investigate the mechanism of transformation-induced fracture in oSMAs from a numerical perspective, a three-dimensional anisotropic rate-dependent constitutive model is proposed. The model is based on the framework of the crystal-mechanics-based constitutive model by Thamburaja and Anand (2001) and features a robust explicit integration scheme to update the constitutive law. Finite element simulations are performed to model the mechanical response and martensite-austenite phase transformation of oSMA wires with triple junction structures. Quantitative analysis is conducted at the microstructural level to interpret the transformation-induced fracture. This model is able to predict the transformation-induced intergranular fracture in oSMA wires and provide insights on the mechanical response, energy absorption and microstructural design of oSMA wires.

Efficient Simulation of Tire Tread Block Dynamics

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ABSTRACT

All forces in vehicle-road contact are transmitted solely via the tire tread: Longitudinal forces - braking/acceleration maneuvers, lateral - cornering, vertical - vibration excitation). Tire tread blocks as the outermost layers of a tire are subject to highly dynamic load and load changes. To be able to simulate tread block dynamics under these transient conditions, efficient models are required. In this presentation I will derive an efficient 3D tread block model with rubber elastic and damping material properties. To optimize calculation time, model order reduction according to Craig & Bampton is applied. The local coefficient of friction between contact nodes and road surface is given in the form of friction characteristics in terms of temperature, sliding velocity and contact pressure; these characteristics originate from in house friction test results. The tread block is following a rolling trajectory, which is approximated to the one provided by the belt in real tires. As validation we vary the width of the tread blocks and compare the results with friction tests performed in our lab: The differences in traction potential between small blocks (winter tire) and wide blocks (summer tires) become obvious - the transmittable coefficient of friction of summer tires is significantly higher on dry road surfaces.

Investigating Dislocation Motion at Ordinary Timescales with Atomistic Simulations and Reaction Rate Theory

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ABSTRACT

To fully utilize the potential of atomistic-to-continuum coupling techniques, their application to finite temperatures and long timescales must be developed. A key challenge in this task is that the success of long timescale atomistic simulations approaches is often specific to the process being examined. This talk will discuss our examination of thermally activated dislocation motion across a field of solutes. First, the accuracy of popular variants of the Harmonic Transition State Theory, as the most common approach, will be examined by comparing predictions to direct MD simulations. Next, the utility of the Transition Interface Sampling will be discussed, as the method was recently shown to be effective for predicting the rate of dislocation-precipitate interactions. For dislocation-solute interactions studied here, TIS was found to be accurate only when the dislocation overcomes multiple obstacles at a time, i.e. jerky motion, and it is inaccurate in the unpinning regime where the energy barrier is of diffusive nature. It will then be shown that the Partial Path TIS method - designed for diffusive barriers - provides accurate predictions in the unpinning regime. The use of the two methods to study the temperature and load dependence of the rate will be presented, where it was found that the Meyer-Neldel (MN) rule prediction of the entropy barrier is not as accurate as it is in the case of dislocation-precipitate interactions. In response, an alternative model will be proposed that provides an accurate prediction of the entropy barrier. This model can be combined with TST to offer an attractively simple rate prediction approach. Lastly, (PP)TIS predictions of the Strain Rate Sensitivity (SRS) factor at experimental strain rates and the predictions will be compared to experimental values.

Multi-Modal Sensor Fusion for State Estimation of an Adaptive Structures Test Bench

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ABSTRACT

In this contribution, we consider the problem of state estimation for adaptive truss structures equipped with a multitude of sensors and actuators spanning different domains [1]. For reliable actuation of such a system, knowledge of the system state, consisting of the building deformation that can be quantified by the spatial deviation of certain building points, is required. However, in a general application, the state is not usually fully measurable, which is why state estimation techniques have to be employed [2]. A scale model of an adaptive truss structure with additional plates is available as an experimentation platform in our laboratory as a scaled version of an actual multi-story building. It is equipped with strain gauges, inertial measurement units and an optical measurement system. The optical measurement system consists of several light emitters, which are attached to the structure's outer faces and point to a remote camera. Using computer generated holograms and a multi-image technique, measurement of the emitter position is achieved with high precision. Sensor fusion is carried out and a complete state estimation is performed. Results obtained by an existing simulation model are experimentally validated on the test bench using actual measurement data. [1] W. Sobek and P. Teuffel, "Adaptive systems in architecture and structural engineering," Proceedings of SPIE, vol. 4330, 2001, pp. 36–45. [2] P. Rapp, M. Heidingsfeld, M. Böhm, O. Sawodny, and C. Tarín, "Multimodal Sensor Fusion of Inertial, Strain, and Distance Data for State Estimation of Adaptive Structures using Particle Filtering", Proceedings of the 2017 IEEE/ASME International Conference on Advanced Intelligent Mechatronics (AIM 2017), 2017.

Pelvic Response of a Total Human Body Finite Element (FE) Model During Simulated Under Body Blast (UBB) Impacts

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ABSTRACT

Under body blast (UBB) events in theater are the cause of many serious injuries sustained by the warfighter to the pelvis, spine, and lower extremities. Injury prediction for UBB events continues to be a challenge due to the limited availability of UBB-specific test studies. This study focuses on the pelvic injury response of the 50th percentile male Global Human Body Models Consortium (GHBMC) FE human body model. The input data used for this study was obtained from testing performed by the Warrior Injury Assessment Manikin (WIAMan) development effort. Evaluation of GHBMC model fidelity and injury response is based on biofidelity targets (corridors) created using pelvis accelerations obtained from experimental testing of UBB-type loading using post mortem human subjects (PMHS). In total, 10 simulations were performed at non-injurious velocities using experimentally recorded seat and floor pulses of 4 m/s. For these simulations, the GHBMC was positioned in a FE vehicle rig seat within the measured tolerances used to position the PMHS for experimental testing. Acceleration data from nodes in the S1 region of the pelvis of the GHBMC were extracted from the simulations. The extracted S1 acceleration data was compared to the biofidelity response corridors (BRCs) for the S1 region of the pelvis developed by the WIAMan program. Additionally, peak force data was extracted from FE cross-sections implemented in localized regions of the pelvis. An analysis was performed using an objective rating method (CORrelation and Analysis, CORA) using the BRC curves. The ± 0.5 and ± 1 SD curves were used for the inner and outer corridor limits, respectively. The average corridor curve was used as the cross-correlation reference. The CORA analysis showed good correlation (70% or higher) of the FE S1 acceleration for all 10 tests when compared to the BRCs. Additionally, the cross-sectional forces from these simulations were compared to pelvic fracture injury risk curves (IRCs) developed for the GHBMC. The peak force values from these simulations exhibited low risk of fracture (below 25%) in these cross-sectional regions. To date, the comparison of full body UBB experimental testing to drive and compare with full body FE simulation metrics for UBB is unique. This data was acquired with the explicit purpose of developing an enhanced capability to predict the risk of injury for mounted soldiers who are subjected to the effects of UBB loading with the goal of enhanced vehicle and soldier survivability.

Identifying and Applying State-Space Models Derived from High-Fidelity Physical Models of Li-ion Batteries

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ABSTRACT

- This paper develops and demonstrates a method to obtain and implement wide-bandwidth, linear, state-space models using binary perturbation. At specified operating conditions (e.g., temperature and state-of-charge), state-space models are identified from physically based battery models using pseudo-random binary sequences (PRBS). These state-space models predict the battery's current-voltage and current-temperature responses over specific frequency ranges. However, because the identified state-space models are accurate over limited frequency ranges, a "stitching" procedure is implemented to develop a single state-space model that is accurate over wide frequency ranges for particular operating conditions. The stitched state-space models, each accurate for particular operating conditions, are gain-scheduled to predict a battery's electrochemical and thermal responses over wide operating ranges. A validation study shows excellent agreement between the low-order gain-scheduled state-space models and the original large-scale physical model. Once validated, the state-space models may be incorporated into model-predictive-control (MPC) algorithms. In the present study, state-space models are identified from large-scale physical models. However, the computational approach is equally applicable to identifying and applying state-space models from experimental investigations.

Isogeometric Design Optimization of Nonlinear 3D Beam Structures for Multi-material 3D Printing and Soft Lattices

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ABSTRACT

In recent years, many new possibilities for design and manufacturing of slender and light-weight structures have emerged through the advancement of advanced and additive manufacturing technologies. Existing and potential applications range from 3D printed micro-structures and meta-materials with slender members, to multi-functional, multi-material and composite structures with locally designed, spatially varying material properties, and to active, smart and self-assembling materials, structures and soft robots with compliant components and tailored large deformation behavior. These new perspectives call for novel design technologies that are capable of optimizing design, shape, and materials of structures subject to large deformations, material nonlinearities, graded and anisotropic materials, functional behavior, etc. In this work, we apply the concept of isogeometric design and analysis for combined shape, topology and design optimization of nonlinear, 3-dimensional beam structures. The mechanics of 3D beams are modelled by the geometrically exact, nonlinear Cosserat rod theory and discretized by an efficient and accurate, NURBS-based isogeometric collocation method [1]. By introducing spline parameterizations not only for the parameterization of geometry, here the centerline positions and cross-section orientations of the rods, but also for material and geometric cross-sections parameters of spatially-variable and functionally-graded rods, e.g. Young's moduli, radii, and layer-ratios of laminate cross-sections, as well as density, we can optimize shape, design and topology of rods and rod structures in a unified isogeometric framework. The resulting nonlinear optimization problem is implemented with analytical design sensitivities using the adjoint method and solved by standard gradient-based optimization methods. The approach is integrated into an isogeometric digital design and fabrication framework from CAD of rod structures, to analysis and optimization of their properties, and to additive manufacturing. We demonstrate our method in several additive manufacturing applications of functional rod structures, including multi-material 3D and 4D printed self-assembling structures [2] and soft, compliant lattice structures [3]. With our isogeometric design-to-manufacturing framework, we show the viability of using of isogeometric analysis and optimization for industrial-type applications. REFERENCES [1] O. Weeger, S.-K. Yeung, M. L. Dunn, "Isogeometric collocation methods for Cosserat rods and rod structures", *Comput. Methods Appl. Mech. Eng.*, Vol. 316, pp. 100–122, (2017). [2] O. Weeger, Y. S. B. Kang, S.-K. Yeung, M. L. Dunn, "Optimal Design and Manufacture of Active Rod Structures with Spatially Variable Materials", *3D Print. Addit. Manuf.*, Vol. 3(4), pp. 204–215, (2016). [3] O. Weeger, N. Boddeti, S.-K. Yeung, S. Kajijima, M. L. Dunn, "Digital Design and Manufacture of Soft Lattice Structures", *Addit. Manuf.*, under review, (2017).

Modeling and Design Optimization of Dynamic Structural Systems under Uncertainty: Application to Epicyclic Gearing

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ABSTRACT

Modeling and design optimization of static mechanical systems has become routine in the development process, while for dynamic systems, challenges remain. Here, these challenges with dynamic structural and mechanical systems will be shown exemplary with epicyclic gearing. Epicyclic gearing has a wide range of applications and can be found in the drive trains of wind turbines, automotive automatic transmissions and automation systems. In this work, numerical optimization methods play a central role and are used to fit model parameters, for uncertainty analysis and to synthesize optimal designs. Parametric models of the dynamic and vibrational behavior are developed and applied to epicyclic gearing. Specifically, the resonance frequencies and frequency-response functions are calculated and used for design performance and limit measures. Results of experimental tests on a benchmark gear system validate these models and identify discrepancies. Numerical optimization is used to fit model parameters to tune values to meet experimental results. Intrinsic uncertainty is handled with interval methods, which bound the uncertain values instead of modeling them with probabilistic distributions. An efficient optimization-based minimization–maximization method is used to carry out uncertainty analyses. These give interval resonance frequencies and interval frequency-response functions, showing the upper- and lower-bound values, which in turn can be used in the design process to guarantee proper performance. Better performance is considered those designs that reduce the vibrational content for an operating case and, therefore, possible noise and fatigue problems. A general design optimization under uncertainty for dynamic systems is shown and used to find optimal designs and applied to a planetary gear system. Though, the same methodology can be used for other applications, such as the energy can also be maximized in cases of energy harvesting. Comparison of optimization methodologies is also shown: zeroth-order algorithms will be contrasted with first- and second-order algorithms as well as with approximation-based optimization in regards to computational effort, repeatability and performance of the optimal design found. Analytical sensitivity analysis allows for added numerical efficiency of the optimization methods. In addition, the sensitivities allow for postprocessing assessments of the optimal results, which assess the effect of the constraint limits (frequency ranges) and uncertainty levels (uncertain stiffnesses) on the objective function. Results are then summarized, providing insight on the design and analysis of dynamical systems and specifically planetary gear trains. This insight can be applied with and without the use of optimization methods, for the latter in the form of design rules.

Quasi-three-dimensional Phase Field Modeling of Martensitic Phase Transformation in Shape Memory Alloys

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ABSTRACT

ABSTRACT The physical and mechanical properties of materials with martensitic phase transformation are significantly influenced by the martensitic transformation process and so-obtained microstructures. In the past two decades, the phase field method has been developed to study the martensitic transformation (MT) behavior and evolution of martensitic microstructure [1-3]. Compared with two-dimensional (2D) simulation, the three-dimensional (3D) modeling of MT has all six components of the stress-free transformation strain. Therefore, all possible variants in MT can be characterized simultaneously by 3D phase field simulation. Further, the complex orientation relationship can be easily revealed in 3D space. However, much more computations are required in 3D phase field simulation. As a consequence, the 3D simulation system (or domain) is restricted to be very small, which is difficult to obtain useful information showing the whole scenario of martensitic transformation. In this study, a quasi-three-dimensional model based on phase field method is developed to reveal martensitic transformation characteristics in shape memory alloys. In the model, we introduce additional degrees of freedom to each node of the plane element in finite element method. So the all six components of the stress-free transformation strain could be expressed. Meanwhile, the order parameter gradient of the vertical direction is used as a new variable to show the angle between the interfacial plane and simulated plane in the microstructure. Thus, the model developed by the present study can well simulate martensitic transformation in arbitrary plane containing all possible variants. Keywords: Phase field; Quasi-three-dimensional modeling; Martensitic transformation; Finite element method References [1] Wang Y, Khachaturyan A G. Three-dimensional field model and computer modeling of martensitic transformations [J]. Acta Mater., 1997, 45: 759. [2] Ke C B, Ma X, Zhang X P. Phase field simulation of effects of pores on B2-R phase transformation in NiTi shape memory alloy [J]. Acta Metall. Sin., 2011, 47: 129 [3] Paranjape H M, Manchiraju S, Anderson P M. A phase field – Finite element approach to model the interaction between phase transformations and plasticity in shape memory alloys [J]. Int. J. Plasticity, 2016, 80: 1

A Mixed RKPM Formulation for Modeling Hydro-Mechanical Damage Processes in Multiphase Porous Media

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ABSTRACT

In the first part of this work, a stabilized Reproducing Kernel Particle Method (RKPM) u-p formulation for hydro-mechanical modeling of multiphase porous media is developed [1]. In this approach, a stable equal-order u-p reproducing kernel approximation for the fluid-saturated porous media is developed by employing a fluid pressure projection method under a variationally consistent nodal integration framework [2] with a least-squares stabilization [3]. It has been shown that the fluid pressure projection method can be naturally integrated within the stabilized conforming nodal integration framework, and thus the non-physical fluid pressure oscillation due to a violation of the inf-sup condition as well as the spurious low-energy modes due to nodal integration can both be eliminated cost-effectively. Next, to capture the complex evolving crack patterns in porous geo-materials, the damage particle method [4] which approximates fractures by a set of damaged particles under the RKPM discretization is introduced. For each damaged particle, a regularized smeared description of the equivalent crack segment at the nodal position is adopted, which avoids spurious damage growth and ensures the objectivity of energy dissipation. The proposed methods are applied to the modeling of landslide and hydraulic fracturing processes. References [1] Wei, H., Chen, J. S., & Hillman, M. (2016). A stabilized nodally integrated meshfree formulation for fully coupled hydro-mechanical analysis of fluid-saturated porous media. *Computers & Fluids*, 141, 105-115. [2] Chen, J. S., Hillman, M., Rüter, M. (2013) An arbitrary order variationally consistent integration method for Galerkin meshfree methods. *International Journal for Numerical Methods in Engineering*, 95(5): 387-418. [3] Puso, M. A., Chen, J. S., Zywickz, E., & Elmer, W. (2008). Meshfree and finite element nodal integration methods. *International Journal for Numerical Methods in Engineering*, 74(3), 416-446. [4] Chen, J. S., Wei, H. (2018). A reproducing kernel damage particle method for multiscale modeling of fracture. *International Journal for Multiscale Computational Engineering* (to be submitted).

A Nonlocal Yield Criterion for Modeling Elastoplastic Deformation in Volume-Compensated Particle Model

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ABSTRACT

Abstract Volume-Compensated Particle Method (VCPM) [1] is a newly proposed nonlocal discontinuous formulation of classical continuum mechanics for mechanical problems with focus on spatial discontinuity. In VCPM, domain of interest is decomposed into discrete material points based on various lattice structures. Each material point interacts with neighboring material points up to certain distance. The interaction between a pair of material points depends on not only the deformations of the two material points themselves, but also the collectively deformation of all their neighbors. Model parameters for calculation of pairwise interactions are derived from material constants, such as Young's modulus and Poisson's Ratio, based on the strain energy equivalence between discontinuous formulation and its continuum counterpart. Since the equation of motion is governed by integro-differential equations, there are no singularity issues in VCPM for problems with spatial discontinuity, such as crack. Discontinuity initiation and propagation are the natural outcome of interaction removal. VCPM has been applied to study various behaviors of solid in the literature. For modeling ductile materials using VCPM, Chen et al. [2] proposed a one-dimensional bond-based critical stretch criterion to model elastoplastic deformation. This criterion only considers specific interaction between one neighboring particle and the particle of interest. The non-local multi-body effect is neglected in this criterion. In this work, a yield criterion for VCPM is proposed to account for the nonlocal effect from all neighbors. This proposed nonlocal yield criterion for each bond depends on not only the deformation of the two material points connected by this bond but also the deformation of all their neighbors. The Atomic Finite Element Method (AFEM) algorithm is implemented to determine the equilibrium state of solids under quasi-static loading. Because of the nonlinearity in an elastoplastic constitutive law, iteration method in combination with incremental loading method is used in the solution procedure. Numerical examples under various loading cases, i.e., uniaxial loading and multiaxial loading, are simulated using the proposed nonlocal yield criterion in VCPM. Good prediction accuracy is established by comparison between VCPM simulation results and ABAQUS simulation results. Reference [1] Chen, H., Jiao, Y., & Liu, Y. (2015). Investigating the microstructural effect on elastic and fracture behavior of polycrystals using a nonlocal lattice particle model. *Materials Science and Engineering: A*, 631, 173-180. [2] Chen, H., Lin, E., & Liu, Y. (2014). A novel Volume-Compensated Particle method for 2D elasticity and plasticity analysis. *International Journal of Solids and Structures*, 51(9), 1819-1833.

Blended B-Spline Construction on Unstructured Quadrilateral and Hexahedral Meshes with Optimal Convergence Rates in Isogeometric Analysis

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ABSTRACT

We present a novel blended B-spline method to construct bicubic/tricubic splines over unstructured quadrilateral and hexahedral meshes for isogeometric analysis. C_1 and (truncated) C_2 B-spline functions are used in regular elements, whereas C_0 and (truncated) C_1 B-spline functions are adopted in boundary elements and interior irregular elements around extraordinary edges/vertices. The truncation mechanism is employed for a seamless transition from irregular to regular elements. The resulting regularity of the blended construction is C_2 -continuous everywhere except C_0 -continuous around extraordinary edges and C_1 -continuous across the interface between irregular and regular elements. The blended B-spline construction yields consistent parameterization during refinement and exhibits optimal convergence rates. Spline functions in the blended construction form a non-negative partition of unity, are linearly independent, and support Bézier extraction such that the construction can be used in existing finite element frameworks. Several examples provide numerical evidence of optimal convergence rates.

Graphene-substrate Interaction and Defects Guided Wrinkling in Graphene

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ABSTRACT

The pattern of wrinkles is governed by the crystallographic planes of the substrates and the defects in the film. In this talk, we report how graphene-substrate interaction as well as commonly seen Stone-Wales defects and grain boundaries (GBs) influence the morphology of graphene on different planes of single crystalline copper substrate. Stone-Wales defects weaken the bending stiffness in graphene, and results in wrinkling along the defect direction. In the presence of GBs, primary wrinkles are always parallel to the GB direction, and there are also secondary wrinkles perpendicular to the GB. In combination with planes of the substrate and the orientation of defects, we demonstrate that we may manipulate wrinkling patterns for possible engineering applications.

A Biophysical Model for Neurodegeneration in the Aging Brain

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ABSTRACT

Biochemical and morphological changes in the aging brain manifest in a progressive cognitive decline, loss of motor control and behavioral changes. We are slowly starting to understand some of the mechanisms of progressive neurodegenerative diseases, such as Alzheimer's disease, Parkinson's disease, and Lewy body dementia, which are generally associated with a propagation of toxic proteins through the brain which cause localized neuron cell death. While the involved misfolded proteins, or prions, such as amyloid-beta, tau, or Lewy bodies, differ for each disease, most neurodegenerative diseases show similar propagation patterns through the brain. Once an initial "toxic seed" appears, prions diffuse through the brain and aggregate in the cortical and subcortical layer. Local aggregation of mature senile plaques leads to the death of neurons and an accelerated spreading of the disease. This progressive neuron death manifests in gray and white matter loss with increasing age and the appearance of clinically known symptoms of neurodegenerative diseases. We present a finite element formulation that couples a reaction-diffusion equation for the prion propagation and classical growth mechanics for the gray and white matter loss in the aging brain. The spreading of prions is characterized by an isotropic propagation through the glial network and an anisotropic diffusion along white matter axons; volume loss due to neuron cell death is driven by the local prion concentration. Based on an anatomically accurate finite element model of the brain, we can reproduce characteristic propagation patterns [1] through the brain and the experimentally observed white and gray matter volume loss over time [2]. Our finite element framework serves as a model system to systematically test propagation mechanisms of individual toxic proteins and to provide new insight into the progression of neurodegenerative disease across temporal and spatial scales. References: [1] Jucker and Walker. Self-propagation of pathogenic protein aggregates in neurodegenerative diseases. Nature 2013. [2] Fjell et al. Critical ages in the life course of the adult brain: nonlinear subcortical aging. Neurobiology of Aging 2013

Generative Design of Lightweight Lattice Structures with Additive Manufacturing Constraints

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ABSTRACT

For the past three decades, topology optimization has been remarkably popular in the engineering design community due to its capability on designing lightweight structures by optimally distributing materials to carry loads. Autodesk Nastran has implemented topology optimization since 2014 and rapidly enhancing its capabilities, including multidisciplinary optimization, hierarchical distributed computing, and various manufacturing method-oriented design. In particular, generating lightweight designs that can be producible by various manufacturing methods is critically important in industry. The topology optimization in Autodesk Nastran can include various manufacturing methods, such as minimum member size, multiple symmetry planes, extrusion, casting, milling, and 3D printing. In particular, 3D printing, or additive manufacturing, becomes an emerging technology as it allows manufacturing complex shapes that were not possible in conventional subtractive manufacturing technologies, such as milling. The current research trend in topology optimization for additive manufacturing focuses on how to design a structure so that the amount of supporting materials can be reduced or removed. However, the technology still remains in the regime of producing solid, isotropic materials. Due to remarkable advances in the additive manufacturing technology, it is now possible to build lattice structures, which involve repetitive patterns of a particular cell shape or type. In fact, lattice structures can be a unique feature for additive manufacturing. It has been demonstrated that lattice structures can reduce the structural weight with the same functionality as with homogeneous materials. This presentation discusses recent developments in topology optimization and lattice structures implemented in Autodesk Nastran. Autodesk Nastran supports lattice structures in topology optimization using Representative Volume Elements (RVEs) so that non-homogeneous tetra element meshes can be used to obtain optimized designs. Multiple design spaces are supported and each design space can have a different lattice material, cell size, member radius, and lattice type. Lattice and non-lattice design spaces can also be mixed. A standard topology optimization is run and the lattice material stiffness is updated every iteration and stresses and stability indexes are computed which reflect actual lattice beam member values. A smoothed STL and optional BREP geometry file are generated at the completion of each analysis which can be meshed using either RVEs (tet10 elements) or shell/beam elements (Autodesk Within) and analyzed for design verification. The presentation will cover the basic theory used in Autodesk Nastran topology optimization including stress and additive manufacturing constraints as well as several examples and classic benchmark problems.

Modelling Particle Segregation in Horizontal Rotating Drums

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ABSTRACT

In several industrial applications, granular materials are often vibrated (shaken) or rotated (sheared) while being processed and transported. As a result, particles or grains with similar characteristics such as the size, density, shape and et cetera typically end up together to find themselves arranged in a range of patterns. This is termed as particle segregation. For example, large particles in bidisperse-in-size mixtures rise towards the free surface when subjected to external vibrations (Brazil-nut effect [1]). On the other hand, small particles form a radial core surrounded by large particles in horizontal rotating drums [2]. Thereby, leading to particle segregation in the radial direction. This presentation focuses on the later scenario, which is particle segregation in horizontal rotated drums. In the past few decades, many experimental and simulational studies have observed and investigated particle segregation in horizontal rotating drums, e.g., [2,3]; however, only a handful of studies have focused on modelling particle segregation in these rotated systems, e.g., [4]. Thereby, as a stepping stone towards predicting particle segregation in mixtures comprising complex granular materials, this work focuses on modelling segregation in bidisperse mixtures comprising of spheres varying in, both, size and density. Similar to our previous modelling work regarding segregation in inclined channel flows [5,6], we will showcase recent advances in utilising the continuum theory for predicting particle segregation in horizontal rotating drums, which will be further validated by utilising experiments or particle simulations. References: [1] A. Rosato, K.J. Strandburg, F. Prinz and R. H. Swendsen, Phys. Rev. Lett. 58 (1987) [2] M. M. H. D. Arntz, H. H. Beftink, W. K. den Otter, W.J. Briels and R.M. Boom, AIChE J. 60 (2014) [3] C. R. K. Windows-Yule, B. J. Scheper, A. J. van der Horn, N. Hainsworth, J. Saunders, D. J. Parker and A. R. Thornton, New J. Phys. 18 (2016) [4] C. P. Schlick, Y. Fan, P. B. Umbanhowar, J. M. Ottino and R. M. Lueptow, J. Fluid Mech. 765 (2016) [5] D.R. Tunuguntla, O. Bokhove and A.R. Thornton, J. Fluid Mech. 749 (2014) [6] D.R. Tunuguntla, T. Weinhart and A.R. Thornton, Comp. Part. Mech. 4(4) (2017)

Contributions of the Osteocyte Canalicular Network to Mineral Homeostasis and Bone's Mechano-Sensitivity

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ABSTRACT

During bone formation, some of the bone-forming osteoblasts stay behind, are walled into the bone matrix and differentiate into osteocytes. These osteocytes use a network of cavities and sub-micrometer wide canals - lacunae and canaliculi - to house their cell bodies and processes, respectively, and to connect with other osteocytes. The importance of the osteocyte network and the corresponding porosity, the osteocyte lacuna-canalicular network (OLCN), has its reason in the ascribed multi-functionality of this structure [1]: (i) mechano-sensation via the detection of the fluid flow through canaliculi; (ii) contribution to mineral homeostasis by exploiting the large surface area provided by the network; (iii) transport of nutrients and signaling molecules. Using a combination of complementary experimental characterization methods, image analysis and computational modeling, we aimed, firstly, to detect spatial correlations between network density and mineral content of the bone to shed light on the networks role in mineral homeostasis, and, secondly, to assess the influence of the network topology [2] on fluid flow through the OLCN. The investigations were performed on human osteons in the femora of healthy middle-aged individuals. Samples were stained with rhodamine and the canalicular network was imaged using confocal laser scanning microscopy and quantified by the canalicular density [3], i.e. the total length of canaliculi per unit volume. The position-dependent mineral content of the same osteons was determined with quantitative backscattered electron imaging. To assess the fluid flow and pressure patterns induced by bone deformation under compression, a model analogous to electric circuits was implemented. A spatial correlation analysis between small regions of interest in the osteons showed that a locally dense canalicular network coincided with an increased mineral content. This accumulation of mineral hints at a mineral reservoir connected to the canalicular network. The fluid flow calculations demonstrated the importance of network density and connectivity for permeability. Particularly striking were the differences in the flow patterns between normal osteons and so-called osteons-in-osteons, where only a few canaliculi bridge the outer part to the inner part formed by remodeling. [1] Kerschnitzki, M., Kollmannsberger, P., Burghammer, M., Duda, G. N., Weinkamer, R., Wagermaier, W., Fratzl, P. (2013), JBMR 28, 1837. [2] Kollmannsberger, P., Kerschnitzki, M., Repp, F., Wagermaier, W., Weinkamer, R., Fratzl, P. (2017), New J.Phys. 19, 073019. [3] Repp, F., Kollmannsberger, P., Roschger, A., Kerschnitzki, M., Berzlanovich, A., Gruber, G. M., Roschger P., Wagermaier, W., Weinkamer, R. (2017), Bone Reports 6, 101.

Intravenous Drug Release from Different Peripheral Catheters

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ABSTRACT

Intravenous therapy is the most common method for administration of medicine or fluid directly into the blood stream using short peripheral catheters (SPCs). Common complication of SPCs' use is thrombophlebitis, a sterile inflammation of the vein wall. Previous studies have shown that up to 80% of patients receiving intravenous therapy develop thrombophlebitis. To date, the biomechanical interaction between the SPCs and the endothelial venous wall has been shown to irritate and activate the endothelial cells thus promote inflammation processes. Very short peripheral catheter (VSPC) is a novel catheter design aimed to reduce the contact between the catheter and the venous wall in order to minimize the biomechanical factor in thrombophlebitis development. The present study aims to explore and compare the dynamics of drug release through the existing SPC and our novel VSPC using experimental and numerical models. An open in-vitro flow loop was designed to simulate drug injection through each of the catheters. Soluble dye injections were recorded and analyzed by image processing methods. Two 3D computational models were created combining a vein section and each of the catheters. The following parameters were measured; (i) Drug washout time; (ii) Drug distribution within the vein; (iii) Drug velocity at the catheter outflow. The results have shown significant dynamic advantage of the VSPC over the SPC; both drug velocity and removal time were faster while injected through VSPC, as well as drug distribution that was located away from the vessel wall when compared to the current commercial SPC. For both of the catheters, increased vein flow rate and injection flow rate resulted in higher proximity of the drug to the vein opposite wall, faster washout time and faster drug velocity at the outflow of the catheter. The results indicate that beyond the bio-mechanical advantage, the VSPC also has a dynamic advantage on the SPC in terms of drug flush profile. Releasing the drug away from the vessel wall can minimize adverse drug effect reaction and potentially reduced the risk for thrombophlebitis.

Representative Models of Polycrystalline and Cellular Materials for Simulation of Properties and Processes at Various Length Scales

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ABSTRACT

The ability to model the structure and properties of a material in a natural way leads to an analysis of structure-property relationships. The mesoscopic models developed as part of these studies can be formed in such a way that geometrical features of the microstructural elements (grains, pores, particles) can be modified with respect to their size, shape, orientation, and spatial position. On the other hand, the properties of the microstructural elements are modeled at atomic scale by application of relevant simulation techniques. The methods developed or adopted here allow one to simulate specific properties and/or processes taking place in the material [1-4]. Three groups of materials are described in these studies: nanometals, particulate composites and open-cell foams. These groups, apparently different from each other when applications are considered, reveal very similar microstructures. Each of the microstructures contains a specific type of interfaces: phase boundary, grain boundary and free surface, respectively. Properties of interfaces and accompanying processes can be simulated at the atomic-scale and the results of such calculations may provide additional data for the design of novel materials. Examples of properties and processes related to the microstructure and structure of interfaces, for a selected group of materials, are presented and discussed here. 1. M. Lewandowska, T. Wejrzanowski, K.J. Kurzydowski, Grain growth in ultrafine grained aluminium processed by hydrostatic extrusion, *Journal of Materials Science*, 43, 2008, 7495–7500 2. J. Skibinski, K. Cwieka, T. Kowalkowski, B. Wysocki, T. Wejrzanowski, K.J. Kurzydowski, The influence of pore size variation on the pressure drop in open-cell foams, *Materials and Design*, *Materials and Design* 87 (2015) 650–655. 3. T. Wejrzanowski, M. Grybczuk, M. Chmielewski, K. Pietrzak, K.J. Kurzydowski, A. Strojny-Nedza, Thermal conductivity of metal-graphene composites, *Materials & Design* 99 (2016) 163-173 4. T. Wejrzanowski, S. Haj Ibrahim, K. Cwieka, M. Loeffler, J. Milewski, E. Zschech, C-G. Lee, Multi-modal porous microstructure for high temperature fuel cell application, *Journal of Power Sources* 373 (2018) 85–94

Performance Engineering – Welcome to the World of FLOPs, Bytes and Cycles!

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ABSTRACT

We consider Performance Engineering (PE) as a structured, iterative process for code optimization and parallelization. The key ingredient is a performance model which provides insights into the interaction between the code and the hardware. The model identifies the actual performance-limiting factors (“bottlenecks”), allowing for a selection of appropriate code changes. Once the impact of the code changes is validated the process restarts with a new bottleneck identified by the performance model. Since this model-based approach provides a thorough understanding of the impact of hardware features on code performance it is also useful in various other areas such as performance reproducibility, performance prediction for future architectures or education and training. We first introduce our PE concept and survey basic “white-box” performance models [1,2] appropriate for performance modelling at the core- and node-level. Choosing a widely used benchmark suite [3] we demonstrate, that automatic “black-box” performance modelling may lead to misleading results if not used with due care. Focusing on selected kernels from sparse and dense linear algebra as well as stencil computations [2] we show various aspects and application scenarios of our “white box” approach. These include data layout considerations for sparse matrix vector product, correct choice of optimization strategies and parameters for stencil computations or identification of performance bottlenecks of building block libraries which are widely considered to be optimal but still can be improved by up to 10x through simple measures. We conclude that code implementation and optimization efforts may greatly benefit in terms of hardware-efficiency, portability and sustainability from using PE in combination with basic white-box performance models. This work is supported by the German Research Foundation (DFG) through the Priority Programs 1648 “Software for Exascale Computing” under projects ESSEX-II (<https://blogs.fau.de/essex/>) and EXASTEEL-2 (<http://www.numerik.uni-koeln.de/14079.html>)

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Multilevel Monte Carlo Methods for Random Vibration Problems

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ABSTRACT

Uncertainty quantification is important for many vibration problems as small variations in model details can have profound effects on the response of a system. To analyse such systems, Monte Carlo methods are widely considered to be computationally too expensive for problems of practical interest, and this has led to the development of many modelling approaches to randomness for vibration problems. These modelling approaches typically lack the flexibility and generality of Monte Carlo methods. In this presentation, we consider the time cost complexity of Monte Carlo methods for eigenvalue problems to show that it is in fact much worse than is commonly thought, and show how the complexity can be conquered by multilevel methods. Multilevel Monte Carlo methods build on the control variate acceleration of Monte Carlo methods by sampling 'coarse' representations of a model, with a limited number of 'correction' samples using the full fidelity model. We present analysis and numerical examples showing that a multilevel approach can make Monte Carlo methods computationally tractable for a range of engineering random vibration problems.

Creep-fatigue-oxidation Crack Growth by Grain Boundary Cavitation

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ABSTRACT

Intergranular cracking of polycrystalline metals in components at high temperatures, under both sustained and cyclic loads, is dominated by various time-dependent mechanisms at the crack tip. In the study, grain boundary cavitation, with cavity growth due to both creep and diffusion, is taken as the major failure mechanism contributing to crack growth. Plane strain finite deformation finite element calculations of mode I crack growth under small scale creep conditions are conducted. The crack growth calculations are based on a micromechanics constitutive relation that couples creep deformation and damage due to grain boundary cavitation. In some calculations, solute-induced grain boundary weakening is modelled by decreasing the critical spacing for grain boundary cavity coalescence. The influence on the crack growth rate of loading history parameters and solute diffusion are explored. Several features of the crack growth behavior observed in creep-fatigue tests naturally emerge; for example, a Paris law type relation is obtained for cyclic loading and the crack growth rate is accelerated by the solute induced grain boundary weakening.

A Combination Rule for Coplanar Cracks under Fatigue and Creep Conditions

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ABSTRACT

It is not uncommon to detect multiple flaws in structures under cyclic loading or at high temperature. A proper prediction of the interaction effect of them is important to prevent a potentially catastrophic failure. In the study, fatigue/creep crack growth simulations, for a plate containing two coplanar surface flaws with both identical and dissimilar sizes, are undertaken in detail by a step-by-step finite element analysis. Combination rules for multiple coplanar flaws provided by fitness-for-service codes are critically assessed for the fatigue/creep failure mode. It is realized that the conservatism contained in existing criteria is highly dependent on the ratio of crack depth to the thickness. With the increase of crack size, as well as the similarity between two cracks, some criteria may lead to a higher risk of non-conservative estimation. Based on the fatigue/creep crack growth life, we suggest a new combination rule and conclude that it always yields a reasonable estimation with necessary conservatism, for various initial crack depths, material constants and relative sizes of two cracks. The difference of conservative degree of combination rules under fatigue and creep conditions is also demonstrated.

A Study on the Influence of Multiple Points Flexible Support Device on Arc-weld Additive Manufacture Process

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ABSTRACT

Layer additive manufacturing is a promising technique for the rapid manufacturing and repair of metallic components. In this field, weld-based rapid prototyping has drawn lots of attention due to the advantages including high productivity, cost saving, and high bonding strength of components. The thermal and residual stress distributions in the welding process have been widely investigated in this study. The thermal and residual stress were also studied by experiment, which are corresponded with the simulation result. Moreover, a multiple-point flexible support device has been novel designed to prevent the deformation of base panel with arc-welded stiffener. Then the validated model was utilized to study when and how big the applied force and release time by the device is proper. The results show that the release time after the end of weld reduce the final deformation, which are not considered in most researches. For instance, when the applied force is 20N and kept for 44s in the numerical example, the deformation in the vertical axis can be eliminated. The validated model was then extended to the case of multi-path multi-layer arc-weld additive manufacture. If the time dependent force transfer from triangular into rectangular, it will provide a more efficient energy consumption. This device will play an important role in the application of welding process of large plate.

Numerical Simulation of Bubble Rising by IMPS-based Multiphase Method

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ABSTRACT

The numerical simulation of bubble rising is challenging since the tracing of deformed multiphase interface. In this paper, a new mesh-less multiphase method is developed based on the IMPS (Improved Moving Particle Semi-implicit) method and applied to simulate the phenomena of bubble rising. In this method, the multiphase system is treated as the multi-density and multi-viscosity fluid. To consider the interaction between particles belonging to different phases, inter-particle viscosity defined by the harmonic mean viscosity is firstly adopted. Then the density smoothing technique is employed to reduce pressure discontinuity crossing the interface to obtain the continuous acceleration and velocity fields. Since the shape of bubble is dominated by the tension on the interface, a contoured continuum surface force (CCSF) model is utilized in the present method. The new multiphase MPS method is validated through comparisons with published numerical data. In particular, the multiphase MPS method is verified against Hysing et al.'s (2009) quantitative benchmark computations of two-dimensional bubble dynamics. Two benchmark cases have been studied by the present method and the evolution of a single bubble rising in a liquid column is concerned. In the first case which corresponds to a low Eötvös number, the present numerical result indicates that the bubble withstands a moderate deformation and ends up in the ellipsoidal regime, while in the second case with a high Eötvös number, the bubble undergoes significant topology change and breaks up eventually. For both cases, good agreements achieved for the benchmark quantities, including circularity, center of mass, and mean rise velocity, which demonstrate the accuracy and stability of the present multiphase MPS method.

Phase-field Approach to Modeling of High-temperature Oxidation of Metals and Alloys

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ABSTRACT

Structural alloys at high-temperatures invariably rely on formation of a slowly growing surface layer of oxide for the necessary oxidation resistance. The transition from internal to external oxidation is often a basis for design of the alloys. During internal oxidation, oxide dilatation is usually severe so that it leads to elastoplastic deformation of the alloy matrix and/or the oxide itself. In addition, the oxide-alloy interface may gradually lose coherency with the growth of oxide precipitation. Modeling of these issues are not trivial and it needs to be resolved prior to realistic simulation of morphological/microstructural evolution of oxide-alloy systems. First, a diffuse-interface electrochemical model is developed to study the fundamental processes during external oxidation in terms of ionic diffusion, diffusion-reaction and the electric field effects. Insights are gained in terms of the applicability of Wagner theory. Furthermore, we develop a thermodynamically consistent phase-field framework to incorporate plasticity and interfacial coherency loss, which paves the way for next-step development of a physics-based phase-field model to study internal oxidation and the transition to external oxidation.

Closure of Reduced Order Models Using Statistical Mechanics Approaches

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ABSTRACT

Reduced order models of multi-scale problems require the modeling of the impact of the unresolved modes on the resolved modes. This is typically referred to as closure modeling. The first part of this talk will provide a brief overview of existing closure modeling approaches in the context of projection-based reduced order models. The second part of the talk will focus on the use of the Mori-Zwanzig formalism (MZ), an idea from non-equilibrium statistical mechanics, as a framework for closure. The MZ formalism offers a mathematically exact framework to derive coarse-grained representations and recasts unclosed terms in the form of a memory integral involving the time history of the resolved variables. As the memory integral is intractable for general problems, we develop a finite memory approximation of the MZ memory kernel and a scale-similarity hypothesis. The outcome of this modeling process is a parameter-free, mathematically-derived closure model. Results are presented for multi-scale problems of transport phenomena, with a focus on evaluating the predictive capability of the ROM.

Calculation Chain for the Sound Calculation of Gearboxes with Multibody Models

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ABSTRACT

The goal of the laboratory of Structural Mechanics and Acoustics at the University of Applied Sciences of Ulm is the simulation of the sound radiation of gearboxes. The classical approach divides the gearbox into three systems: 1. The inner parts like shafts, gears and bearings as a multibody simulation model 2. The gearbox housing as a finite element model 3. The radiating housing surface and the surrounding fluid as an acoustic boundary or finite element model. With that concept, the exciting bearing forces are calculated with the first model. Those exciting forces (transferred into the frequency domain) are the input for a frequency response analysis of the gearbox housing. The results are the surface velocities as a boundary condition for the third acoustic model for the calculation of the radiated sound. The mayor difficulty here consists in the long computation time and the neglect of the interaction between the inner parts and the housing. One way to solve that problem is proposed in [1] by using a reduced order model of the housing in the multibody model. That means that the first two systems are connected in one multibody model so that the surface velocities of the radiating housing are calculated in the time domain. As the sound calculation is more efficient in the frequency domain, a FFT is applied to the velocities. Additionally this contribution includes further optimizations of the gearbox model needed for a higher calculation efficiency. Usually the gears are modelled with complex and time consuming 3D contacts. Various authors already presented suitable solutions for modelling gear pairs with generalized force elements that rely on pre-calculated stiffnesses [2]. The same concept is applied to the bearings where the manufacturer typically provides the stiffness maps. In order to validate this approach the interaction between the housing and the bearings is measured with a unique setup of newly developed sensors. This also allows determining the path contributions of each bearing to every radiating surface point via an Operational Transfer Path Analysis. To sum it up, a new approach for a time-efficient multibody gearbox model will be presented alongside with the according experimental validation techniques. [1]: Kirsch, Wegerhoff, Jacobs: Prognosemethodik für die Schalleistung von Getrieben während der Konstruktionsphase, FVA Nr. 587 II, Frankfurt, 2016 [2]: Palermo, Mundo, Hadjit, Desmet: Multibody element for spur and helical gear meshing based on detailed three-dimensional contact calculations, Mechanism and Machine Theory 62 (2013) 13-30

Multi-grain Phase-field Model for Ferroelectric Materials

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ABSTRACT

Ferroelectric materials with a perovskite crystal structure are widely used in applications like actuators, fuel injection systems, and sonar applications. The most widely spread commercial material is $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ due to its outstanding electromechanical properties and large temperature range for applications. Based on the Landau-Ginsburg-Devonshire (LGD) thermodynamic theory, Haun et al. was able to describe lead-based composition material. However, many effects do still not fit the prediction of LGD and need further investigation. One such phenomenon happens near the so-called morphotropic phase boundary (MPB). The MPB is hereby a compositional area in the phase diagram where the crystal structure changes from the tetragonal phase to the rhombohedral phase without changing the formulae type ABO_3 . In the vicinity of the MPB, the $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ -material passes through a minimum in the coercive field and a maximum in the obtainable strain. The experimentally determined strain is much larger than theoretically predicted. The reason for this discrepancy is the complex interplay of the different strain mechanisms and field induced phase transitions dependent on grain orientation [1]. For adjusting the theoretical prediction to the macroscopic observations, one possible approach [2] relies on measurements of the spontaneous strains for different phases using diffraction techniques. As a result, phase-dependent electrostrictive appliances QT and QR for tetragonal and rhombohedral phases are obtained. The aim of this work is to combine the LGD theory with a phase-field approach incorporating continuum mechanics of the elastic field [3] and to enable simulations of polarization domains inside the grain structures of different simultaneously present crystalline phases. In this presentation, the theory and fundamental model equations are explained and simulation results are shown in comparison with experimental data. [1] Hinterstein, M., Hoelzel, M., Rouquette, J., Haines, J., Glaum, J., Kungl, H. & Hoffman, M.: Interplay of strain mechanisms in morphotropic piezoceramics. *Acta Mater.* 94, 319 (2015). [2] Franzbach Daniel J, Seo Yo-Han, Studer Andrew J, Zhang Yichi, Glaum Julia, Daniels John E, Koruza Jurij, Benan Andreja, Mali Barbara, and Webber Kyle G. Electric-field-induced phase transitions in co-doped $\text{pb}(\text{zr}_{1-x}\text{tix})\text{o}_3$ at the morphotropic phase boundary. *Science and Technology of Advanced Materials*, 15, 02 2014. [3] Daniel Schneider, Felix Schwab, Ephraim Schoof, Andreas Reiter, Christoph Herrmann, Michael Selzer, Thomas Boehlke, and Britta Nestler. On the stress calculation within phase-field approaches: a model for finite deformations. *Computational Mechanics*, pages 1–15, 2017.

Improved Workflow for Unsupervised Multiphase Image Segmentation

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ABSTRACT

Quantitative image analysis often depends on accurate classification of pixels through a segmentation process. However, imaging artifacts such as the partial volume effect and sensor noise complicate the classification process. These effects increase the pixel intensity variance of each constituent class, causing intensity values of one class to overlap with another. This increased variance makes threshold based segmentation methods insufficient due to ambiguous overlap regions in the pixel intensity distributions. The class ambiguity becomes even more complex for systems with more than two constituent classes. We present an image processing workflow that improves segmentation accuracy for multiphase systems. First, the ambiguous transition regions between classes are identified and removed, which allows for global thresholding of single-class regions. Then the transition regions are classified using a distance function, and finally both segmentations are combined into one classified image. We present two methodologies for identifying transition pixels that use the results of a steerable filter and local deconvolution of the image pixels. We demonstrate on a variety of synthetic images that the misclassification errors and area differences calculated between each class of the synthetic images and the resultant segmented images range from 0.69-1.48% and 0.01-0.74%, respectively, showing the accuracy of this approach. We also present results demonstrating that this approach can accurately segment x-ray microtomography images of moist granular media using these computationally efficient methodologies.

Advances in Solution Schemes for Nonlinear Multiphase Flow and Transport in Porous Media

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ABSTRACT

This presentation consists of two developments. The first topic is on an approximate Jacobian nonlinear solver. This approach has been shown to outperform the two stage or CPR preconditioners conventionally designed for several multiphase flow problems. Here, we present an alternative to two-stage preconditioning (or CPR) for solving the aforementioned monolithic system after Newton linearization. This method relies upon an approximation in the nonlinear, fully discrete, variational formulation resulting in decoupling of the DOFs and consequent approximate Jacobian construction. The resulting linear system is easily reduced to one in pressure (reference phase) degrees of freedom (DOF) only circumventing the need for specialized preconditioners. Further, the linear system has fewer DOF owing to the elimination of saturations (or concentrations). The second topic is a space-time domain decomposition approach using the enhanced velocity mixed finite element method. This approach allows for non-matching subdomain discretizations both in space and time for non-linear flow and transport problems that are locally mass conservative. In order to accurately resolve these non-linearities, it is often necessary that a small time-step size be used during the numerical solve. Consequently, this approach is computationally prohibitive. We present a space-time domain decomposition approach that overcomes these difficulties.

Error Estimates of the Fixed Stress Iterative Scheme for Coupling Flow with Geomechanics

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ABSTRACT

Coupled poromechanical processes arise in various applications in the subsurface. Wellbore collapse, sand production, reservoir compaction and surface subsidence are examples of different classes of problems where fluid flow and geomechanics mutually affects the displacements and pressures in the ground. Thus, conducting a coupled porous and solid deformation analysis plays a critical role in simulating the field behavior. However, large scale modeling of coupled processes is a computational challenge that has been historically considered very complicated. Iterative methods for solving coupled flow and geomechanics have gained popularity in the last two decades for their simplicity and numerical efficiency. They are based on decoupling the equations using an intermediate sub-step; the flow, or the geomechanics, equations are solved first to obtain a solution for the other problem. This procedure is repeated at each time step until the solutions of the two problems converge to an acceptable tolerance. In this work, we consider a fixed- stress split algorithm to decouple the displacement equations from the flow equations for a large scale Biot system. The pressure flow equations are discretized by a mixed finite element method (MFEM) and the elastic displacement equations are discretized by a continuous Galerkin scheme (CG). A priori error estimates are derived with the expected order of accuracy provided the algorithm is sufficiently iterated at each time step. These error indicators are implemented in a large scale reservoir simulator (IPARS). A posteriori error estimators are also derived and implemented to help choose suitable mesh refinement. Numerical simulations are presented to confirm the theoretical results.

Gas Transport through the Pore Space of Seasonal Snow

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ABSTRACT

Over half of the Earth's total land surface area in the northern hemisphere can be covered by snow in the winter. This large expanse of snow cover impacts many climate-sensitive phenomena including surface-atmosphere exchange processes, ground thermal regime, and water resources. Knowledge of the fundamental properties of seasonal snow is important for analysis in all of these areas. While transient models of gas diffusion through pore space of snow have been made, direct measurements of the gas diffusion through snow's complex pore space are lacking, despite a need for these measurements to ensure model accuracy. In this study we developed an advection-diffusion transport model of gas movement through seasonal snow and we present results from multiple experiments conducted on glass beads, used to verify correct interpretation of the transport physics. We further utilize the verified model, along with the first ever in-situ measurements of gas diffusion through snow, to describe the effective diffusivity of six different seasonal snow types, distinguished from one another by characteristic microstructure. Our transport model incorporates previous work on snow ventilation to account for subsurface air flow that is caused by wind flowing over features in the snow surface. Results suggest that steady winds blowing over surface roughness features can impact the transport of gas through the pore space of snow and therefore must be accounted for within transport models. After accounting for wind, our model and measurement results indicate a large discrepancy between our values and values from two common theoretical derivations of effective diffusivity in snow that are based mainly on measured density. Unlike derivations based on density, our results show that complex (non-spherical) crystal shape leads to interstitial gas diffusivity that is not captured by existing theoretical equations in part due to the original assumptions of isotropy and spherical ice grains. These results provide improved guidance for estimates of gas diffusivity in seasonal snow, to be used in surface-atmosphere gas-flux models. The transport model and experimental approach used in this work could be adjusted and incorporated into future studies of gas transport properties of other porous materials that are exposed to an advective flow.

Consistent Finite-Element Schemes for Subsurface Flow Simulation

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ABSTRACT

Computational simulation of coupled flow and transport in porous media plays an important role for reservoir development and management in the oil and gas industry, for predicting the fate of contaminants in groundwater formations as part of soil remediation efforts, and for studying the efficacy of geologic sequestration of carbon dioxide as a way of reducing emissions into the environment. Because these are important applications and can also incur significant capital expenses, the quest for accurate numerical prediction is ongoing. Computational models for these applications involve the coupling between a discrete approximation to the fluid velocity (or fluid velocities in case of multiphase-flow problems) and the discretized transport equation. In addition to carefully selecting computational approaches for each sub-problem – i.e., the appropriate schemes for velocity and transport discretizations – based on accuracy, speed and robustness, coupling these two computational approaches adds another layer of complexity and restrictions. In particular, the issue of mass conservation (both global and local) is often at the forefront, as spurious mass imbalances not only lead to inaccuracies but can also trigger numerical instabilities, especially for nonlinear multiphase-flow problems. Being heterogeneous and geometrically complex, geologic models and groundwater formations are best discretized by unstructured meshes. While the continuous finite-element method is a natural computational approach for handling such configurations, it has often been dismissed as a technique for simulating flow and transport because it lacks the proper mass-conservation properties. In particular, numerous statements have been made in the literature regarding the lack of conservation at the element level, i.e., mass imbalances that occur when summing up fluxes around element facets. While these statements are true, they fail to take a holistic approach and consider the coupled problem as a whole. We show that, as long as the flow equations and the transport equations are discretized consistently both in time and space, the continuous finite-element method can be a robust, accurate, and practical computational technique for solving these coupled flow and transport problems.

Topology Optimization with the Stress-based Finite Element Method of Solving the Equilibrium Problem

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ABSTRACT

Abstract: The topology optimization problem for two-dimensional statically loaded structures has been considered. In contrast to commonly used approaches where the displacement field is applied as the main unknown variable in the solution of the equilibrium problem, the stress field has been utilized as the main unknown variable in the present paper. The optimization problem has been solved by the solid isotropic material with penalization (SIMP) approach. Several cases of structures optimized by applying both the displacement and stress-based finite element methods have been analyzed. The results obtained by the two methods have been compared. The optimization problem has been formulated so that the minimum of compliance is to be found provided that the material volume is constant and the stress field is the solution of the linear equilibrium problem [2,1]. The main differences in the present approach is that the compliance functional depends on the stress tensor directly and the equilibrium problem has been solved by minimization of complementary energy on the set of statically admissible stress fields. The equilibrium equations have been fulfilled inside the design domain by means of the Airy stress function which has been approximated using the rectangular element with 16 degrees of freedom which guarantees continuity of the approximated function and its first derivatives [3]. To satisfy the stress boundary conditions that have a form of linear constraints for degrees of freedom, the Lagrange multiplier technique has been applied [3]. A number of optimization tasks has been analyzed by the proposed technique and the well known approach presented in [1] where the rectangular element with 8 degrees of freedom has been applied. A significant smaller number of iterations needed to get the solution has been observed in the case of the present method. However, a single iteration takes more time in the case of stress-based approach where the calculations are more complicated. A sharper image of the optimized structure has been obtained by the stress-based method in the most of the considered cases. References [1] Andreassen E., Clausen A., Schevenels M., Lazarov B. S. and Sigmund O., Efficient topology optimization in MATLAB using 88 lines of code, *Struct. Multidisc. Optim.*, 43 (1), 1-16 (2011). [2] Bendsoe M.P., Sigmund O., *Topology Optimization*, Springer Verlag, Berlin, 2003. [3] Wieckowski Z., Youn S.K., Moon B.S., Stress-based finite element analysis of plane plasticity problems, *Int. J. Numer. Meth. Eng.*, 44, 1505-1525 (1999).

Hybrid Nonlinear Finite Elements and Peridynamics Using a Node-Based Force Scheme

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ABSTRACT

A hybrid peridynamics/finite element method is discussed in which nonlinear finite elements (with a bi-linear stress-strain model) are used with a bond-based peridynamics method. In this approach, the peridynamics nodes are coincident with the finite element nodes and a force-blending scheme is used [1]. At each time step, both the peridynamic and finite element force is computed at each node, though peridynamics is only used at the onset of damage. The peridynamics constant is based on the tangent modulus of the surrounding finite elements, rather than the modulus in the linear region. A damage-adjusted bond breakage method [2] is used along with force-damping [3]. Damage-based blending is used at low-levels of damage, essentially before a full fracture surface separates a horizon. With this approach, a damage-dependent linear combination of the finite element force and peridynamic force is used at each node to smooth the transition from local to nonlocal model and to continue to capture the nonlinear effects. The main advantage of this approach is that using finite elements in the bulk is more accurate than peridynamics, while of course peridynamics is most useful for fracture modeling. Further, nonlinear finite element material models are more established than equivalent peridynamics models. Several numerical results demonstrate the efficacy of the method. [1] Wildman, Raymond A., James T. O'Grady, and George A. Gazonas. "A hybrid multiscale finite element/peridynamics method." *International Journal of Fracture* (2017): 1-13. [2] Ha, Youn Doh, and Florin Bobaru. "Characteristics of dynamic brittle fracture captured with peridynamics." *Engineering Fracture Mechanics* 78.6 (2011): 1156-1168. [3] Silling, Stewart. "Introduction to Peridynamics." *Handbook of Peridynamic Modeling*. Eds. Bobaru, Florin, et al.. CRC Press, 2016.

Scale Resolving Simulations of the Aerodynamic Flow around an Airfoil Using a Lattice Boltzmann Method

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ABSTRACT

Scale resolving simulations based on the Lattice Boltzmann method are used to predict the flow around a NACA airfoil profile. The objective of this work is to predict the complex unsteady aerodynamic flow over clean and iced airfoils. The correct prediction of the maximum lift coefficient is important for safety reasons but is very challenging for iced airfoils since the flow is highly turbulent, three-dimensional and local separations may occur over the complex ice shapes. For this purpose, a hybrid RANS / LES model as well as wall-modeled LES are used with the Lattice Boltzmann Method (LBM). The LBM is an attractive alternative to the traditional Navier-Stokes approach due to its compact nature which makes it particularly suited for massively parallel simulations. It thus enables the study of geometrically and physically complex flows using scale resolving simulations at lower cost. The D3Q19 lattice model is used together with a regularized BGK collision model [1]. The LBM is applied on a multi-domain uniform mesh. An immersed solid boundary method is used to handle the connection between the volumetric mesh in the fluid and the surface mesh defining the solid domain. A reconstruction method of the distribution functions at the boundary nodes is used based on the evaluation of the macroscopic variables. Using a uniform grid, it would be too expensive to explicitly resolve the boundary layer. Therefore a wall model is implemented to evaluate the velocity at the boundary nodes. In this context, a Detached Eddy Simulation (DES) model is implemented based on the Spalart-Allmaras turbulence model. The behavior of this RANS turbulence model in the boundary layer is taken into account in the wall model. DES calculations of the flow around a clean NACA airfoil are conducted in order to validate the methodology. Wall-modeled LES of the clean airfoil are also performed. Several angles of attack are considered to reproduce the polar curve of the NACA profile. Light icing on the airfoil is taken into account by adding a roughness term in the wall model whereas horn type icing is explicitly resolved. Calculations are validated by comparison with experimental results and references of lift and drag coefficients as well as pressure coefficient distributions on the airfoil. [1] Latt, J., Chopard, B., Sep. 2006. Lattice Boltzmann method with regularized pre-collision distribution functions. *Mathematics and Computers in Simulation* 72 (2-6), 165–168.

Dislocation-based Crystal Plasticity Modeling of Dynamic Ductile Failure

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ABSTRACT

A framework for dislocation-based viscoplasticity and dynamic ductile failure has been developed in (Nguyen et al., 2017) to model high strain rate deformation and damage in single crystals and polycrystals. The rate-dependence of the crystal plasticity formulation is based on the physics of relativistic dislocation kinetics suited for extremely high strain rates. The damage evolution is based on the dynamics of void growth, which are governed by both micro-inertia as well as dislocation kinetics and dislocation substructure evolution. An averaging scheme is proposed in order to approximate the evolution of the dislocation substructure in both the macroscale as well as its spatial distribution at the microscale. Additionally, a concept of a single equivalent dislocation density that effectively captures the collective influence of dislocation density on all active slip systems is proposed here. Together, these concepts and approximations enable the use of semi-analytic solutions for void growth dynamics developed in (Wilkerson and Ramesh, 2014), which greatly reduce the computational overhead that would otherwise be required. The resulting homogenized framework has been implemented into a commercially available finite element package, and a validation study against a suite of direct numerical simulations was carried out. Lastly, polycrystalline samples are studied at the mesoscale level through the explicit resolution of each grain, i.e. resolving each individual grain size, shape, and orientation, in a representative volume element. In these polycrystal simulations, failure naturally localizes along grain boundaries of particular misorientation in agreement with recent experimental observations, e.g. (Brown et al., 2015). Nguyen, T., Luscher, D.J., Wilkerson, J.W., "A dislocation-based crystal plasticity framework for dynamic ductile failure of single crystals," *J. Mech. Phys. Solids*, 108:1-29, 2017. Wilkerson, J.W., Ramesh, K.T., "A dynamic void growth model governed by dislocation kinetics," *J. Mech. Phys. Solids*, 70:262-280, 2014. Brown, A.D., Wayne, L., Pham, Q. et al., "Microstructural effects on damage nucleation in shock-loaded polycrystalline copper," *Metall. and Mat. Trans. A*, 46:4539, 2015.

Toward Validation of Meshfree Modeling of Underbody Blast Experiments

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ABSTRACT

In the last twenty years, research has been conducted to determine the predominant factors affecting the impulse imparted by a buried charge to an overhead structure. It has been shown that the blast-loading environment is a function of many factors including the explosive type, configuration, mass, and depth of burial, the soil characteristics, and the distance between the ground surface and the target structure. As a part of this research, the U.S. Army Engineer Research and Development Center (ERDC) has focused considerable attention on understanding the relationship between a buried explosive charge and the surrounding geologic/soil materials and advancing our ability to predict these soil/explosive phenomena in high performance calculations. Through this research effort, it was found that there was a lack of consistent, repeatable, highly instrumented experiments to validate the computational simulations. This presentation discusses the meshfree modeling and results of recent underbody blast experiments with rigid and deformable targets that the ERDC conducted for software validation. The problem setup consists of a target at a given standoff from the ground surface with the explosive buried below the soil surface. The modeling involves significant mixing interactions of soils, explosive detonation products, air, and metal components. Comparisons of total impulse, deformation where applicable, and soil stress and velocity were made of the simulation and experimental results. The results obtained from this research provided detailed insight into the blast load environment created in a shallow-buried underbody blast event. This work also provided much needed critical validation experiment data that can be utilized to gain confidence in the models to predict the loading and deformation from a realistic underbody blast test event.

Reliable Thermophysical Property Data of Metal Systems for Integrated Computational Materials Design and the Next Generation Reporting Standard ThermoML 5.0

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ABSTRACT

The electronic availability of thermophysical property data in a well-structured machine-readable format is one of the cornerstones of a robust infrastructure for materials development. With Integrated Computational Materials Engineering (ICME) such a system promises substantially faster development and deployment of advanced materials at a fraction of the cost we face today. Equally important for a collection of well-characterized experimental thermophysical property data are their provenance and a clear statement regarding their quality quantified in statements of uncertainty. The Thermodynamics Research Center (TRC) within NIST has, for the last four years, actively engaged in addressing this challenges for the thermophysical property data for metals and alloys. This talk covers the progress in the continuous development of the free, publicly available NIST/TRC online resources (http://trc.nist.gov/metals_data) for metals and alloy data. It will include the progress made in capturing and structuring all relevant information from open literature into well-vetted datasets that can now be accessed and used via the Web through a human-oriented or computer-oriented (API) interface. Increased need for interoperability between data providers and data users also demands a data storage and exchange protocol for experimental and critically evaluated thermophysical and thermochemical property data. ThermoML is an XML-based IUPAC standard and the latest revision is a significant update to a more modern XML usage and adds the necessary elements for the representation of metal-based systems while maintaining compatibility to the traditional representation for organic-based systems. The latest efforts to expand the domain of applicability for this data communication standard, the active IUPAC project with the title "ThermoML-2017 REVISION OF AN XML BASED IUPAC STANDARD FOR THERMODYNAMIC PROPERTY DATA" will also be discussed.

Computational Fluid Mechanics without Equation Solver: A Meshless Point Collocation Method for Incompressible Navier-Stokes Equations

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ABSTRACT

Abstract: We developed a very efficient numerical framework for non-stationary, incompressible Navier-Stokes (N-S) equations. The framework does not require an equation solver. We use strong form meshless collocation method to compute spatial derivatives on point cloud [1] and combine the flexibility of this method with the robustness of mesoscopic methods (we use Lattice-Boltzmann LB [3]) to numerically solve Poisson equations of mass conservation. We use explicit time integration schemes (Euler and 4th order Runge-Kutta RK4) with the critical time step determined using Gerschgorin circle theorem [2]. Application of this theorem facilitates rapid ("on-the-fly") time step computation. We implemented the proposed framework using MATLAB programming language and applied it to flow (incompressible N-S) equations in both their primitive variable (u-p) and velocity-vorticity (u- ω) formulations. The latter has been extended in 3D by using the vector potential method. We used lid-driven cavity problem in 2-D (rectangular domain) and 3-D (cubical domain) as benchmarks. The proposed framework can be easily parallelized, which makes it particularly attractive for GPU implementation. Furthermore, the Poisson type equation(s) can be solved through the traditional mesh-based methods, such as the Finite Element (FE) and the Finite Volume (FV), by using identical nodal distributions. The resulting linear systems are positive definite, diagonally dominant and symmetric and, therefore, robust iterative solvers (with appropriate preconditioners) have been developed over the past 30 years, ensuring a fast and accurate numerical solution. References [1] G. C. Bourantas, B. L. Cheesman, R. Ramaswamy, I. F. Sbalzarini. Using DC PSE operator discretization in Eulerian meshless collocation methods improves their robustness in complex geometries *Computers & Fluids* 136 285-300 (2016). [2] Isaacson, E. and Keller, H. B. 1966. *Analysis of Numerical Methods*, New York, Wiley, Library of Congress Catalog Card Number: 66-17630. [3] Chen S, Doolen GD. Lattice Boltzmann method for fluid flows *Annual Review of Fluid Mechanics* 30: 329-364 (1998).

Hierarchical Elastoplasticity of Bone: Theory, Algorithm, and Experimental Validation

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ABSTRACT

Introduction Bone is characterized by a hierarchically organized microstructure, exhibiting „universal” organizational patterns, whose „dosages”, however, vary between different species, organs, and anatomical locations - resulting in a great variety of mechanical properties. This complex internal structure leads to a necessity of taking into account all the different hierarchical components - some of which behave plastic - in order to explain the overall mechanical elastoplastic response of the bone. We here use a multiscale micromechanical model to predict the resistance to failure under mechanical load - the bone strength - based on the mechanical properties and volume fractions of its three elementary constituents: mineral, collagen and water. Methods Building on an earlier micromechanical explanation of bone strength (1) as well as on recent advances gained in the mechanics of crystalline structures (2) we developed an extended elastoplastic multiscale continuum micromechanics model for bone, based on the concept of concentration and influence tensors for eigenstressed microheterogeneous materials (3). The hierarchical organization of bone is considered in terms of six representative volume elements: cortical bone with cylindrical vascular pores, extravascular bone matrix with spherical lacunae pores and extracellular bone matrix consisting of cylindrical, mineralized collagen fibrils embedded into an extrafibrillar matrix, as well as wet mineral foam. The mineral is represented as an infinite number of cylindrical mineral phases oriented in all spatial directions interacting with spherical, water-filled pores within the extrafibrillar and the fibrillar space. The sole source of elastoplasticity lies in mutual sliding between those mineral phases, which are characterized by non-associated Mohr-Coulomb elastoplasticity; while the molecular collagen phase fails in a brittle manner, according to a Rankine criterion. Upscaling of these processes from the nano to the macroscale was made possible by a novel variant of the so-called return-map algorithm. Results The model is able to accurately predict the experimentally determined strength of bone tested in uniaxial tension and compression. While the strength is governed by the failure of the mineral during compression, the collagen failure defines the tensile strength. Furthermore, the sequence of plastic events and the stresses and strains can be determined across all hierarchical levels, illustrating the influence of the different components on the overall mechanical behavior of bone. References (1) Fritsch, Hellmich and Dormieux (2009), *Journal of Theoretical Biology* 260(2):230–252 (2) Morin, Vass and Hellmich (2017), *International Journal of Plasticity* 91:238–267 (3) Pichler and Hellmich (2010), *Journal of Engineering Mechanics* 136(8):1043–1053

A Generalized Algorithm for Finite Strain Plasticity

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ABSTRACT

We introduce a generalized numerical algorithm for elasto-plastic problems at finite strains. Based on the Karush-Kuhn-Tucker system characterizing finite elastoplasticity, the presented algorithm solves linearized sub-problems iteratively. This linearization scheme may be extended to non-classical formulations of elastoplasticity, in which the plastic variables are not treated as internal variables. The generalized algorithm is compared to the classical Return Mapping Algorithm (RMA) with respect to the structural set-up and the computational effort. Especially some restrictions of the Return Mapping Algorithm in its classical form are pointed out. These can be overcome by means of the proposed method. Finally, the Generalized Plasticity Algorithm (GPA) and its convergence are tested by solving some benchmark problems.

Geometric Implications for Stress Concentration in Miura Origami

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ABSTRACT

Origami principles have inspired foldable and reconfigurable thin-sheet structures for various engineering applications. At small length scales origami is well suited for creating metamaterials with adaptable and tunable properties. Analyzing stress distributions in the thin-sheet structures is important for improving robustness by predicting and potentially preventing failures. Additionally, origami systems which are intentionally designed to localize stresses can fail and collapse in predictive and preferred failure sequences [1]. In origami metamaterials, the controlled failure sequences could further expand the programmability and adaptability of the hierarchical systems. This work explores the Miura-ori pattern because it has attracted tremendous attention for its mechanical properties. The pattern is developable, rigid foldable and flat foldable, and can achieve negative Poisson's ratios, high stiffness-to-weight ratios, and tunable properties [2]. The Miura-ori typically fails at the origami vertices. These failures can be partly attributed to stress from folding a sheet with finite thickness, however, the restrictive geometry and sharp corners of the pattern also induce high stress concentrations at the vertices [3]. To realize the relationship between stress concentration and geometry of the Miura-ori, a finite element model where shells and rotational hinges are employed, simulates the stress distribution in the origami (idealized as zero-thickness). Three distinct loading cases are studied for the origami and the different geometric parameters of the Miura-ori are systematically varied. The panel side ratios (height/width), panel vertex angle of the Miura, as well as the fold angle all influence the load paths and stress distributions in the origami. [1] Ma J., and You Z. (2013). Energy absorption of thin-walled square tubes with a prefolded origami pattern-Part I: Geometry and numerical simulation. *Journal of Applied Mechanics*, 81: 011003. [2] Schenk, M., and Guest, S. D. (2013). Geometry of Miura-folded metamaterials. *Proceedings of the National Academy of Sciences*, 110(9), 3276–3281. <https://doi.org/10.1073/pnas.1217998110> [3] Witten, T. A. (2007). Stress focusing in elastic sheets. *Rev. Mod. Phys.*, 79(2), 643–675. <https://doi.org/10.1103/RevModPhys.79.643>

Using Graphs to Quantify Energetic and Structural (Dis)order in Organic Thin Films

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ABSTRACT

The nanomorphology of polymer blend thin films critically affects performance especially in organic solar cells. However, many aspects of the underlying physics linking morphology to performance are still poorly understood. Furthermore, there is increasing evidence that atomic organization can hold the key to efficient charge transport within organic electronic devices. In order to fully capitalize on these recent evidence, there is a need to quantify the atomistic and energy features of morphologies with respect to basic steps of photovoltaic process. In this work, we take advantage of recent advances in molecular dynamic simulations and quantify atomic-scale morphological aspects of the thin films. Specifically, we present a graph-based technique that allows quantifying the point-cloud data (MD). In our approach, we first convert the point cloud data from atomistic simulation into a labelled, weighted, undirected graph and then use standard graph-based algorithms to calculate and quantify morphology features. The conversion of the CGMD-data into a graph preserves all the topological and geometric information about the internal structure, and local connectivity between individual atoms/beads (along and across the polymer chains). More importantly, the edges between individual beads on CGMD can be labelled by Euclidean distance, energy difference or hopping rate. Our method provides hierarchical information about the charge paths that a hole/electron needs to take to reach the electrode (path length, travel time, fraction of intra-molecular hops, path balance). We showcase capabilities of our approach by analyzing coarse grained molecular simulations of several oligothiophene blends. We present how graph-based method allows to provide quantitative insight into the origins of few orders of magnitude difference in mobility.

Computing Eddy-driven Effective Diffusivity Using Lagrangian Particles

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ABSTRACT

A novel method to derive effective diffusivity from Lagrangian particle trajectory data sets is developed and then analyzed relative to particle-derived meridional diffusivity for eddy-driven mixing in an idealized circumpolar current. Quantitative standard dispersion- and transport-based mixing diagnostics are defined, compared and contrasted to motivate the computation and use of effective diffusivity derived from Lagrangian particles. The effective diffusivity is computed by first performing scalar transport on Lagrangian control areas using stored trajectories computed from online Lagrangian In-situ Global High-performance particle Tracking (LIGHT) using the Model for Prediction Across Scales Ocean (MPAS-O). The Lagrangian scalar transport scheme is compared against an Eulerian scalar transport scheme. Spatially-variable effective diffusivities are computed from resulting time-varying cumulative concentrations that vary as a function of cumulative area. The transport-based Eulerian and Lagrangian effective diffusivity diagnostics are found to be qualitatively consistent with the dispersion-based diffusivity. All diffusivity estimates show a region of increased subsurface diffusivity within the core of an idealized circumpolar current and results are within a factor of two of each other. The Eulerian and Lagrangian effective diffusivities are most similar; smaller and more spatially diffused values are obtained with the dispersion-based diffusivity computed with particle clusters.

Validation of Multiscale Designer against AS4/8552, IM7/8552, and IM7/EP2202 NCAMP Data for Unidirectional Product Forms

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ABSTRACT

Multiscale Designer is a stochastic multiscale material modelling framework that seeks to develop highly accurate and computationally efficient multiscale material models which rely on minimal testing. Multiscale Designer is a part of the Altair HyperWorks suite of tools. The presentation will first overview the methodology used to develop multiscale material models for unidirectional product forms from minimal testing; typically [0] tension/compression, [90] tension/compression, and [45/-45] tension. The second part of the presentation will present validation results for multiscale material models developed for AS4/8552, IM7/8552, and IM7/EP2202 NCAMP unidirectional materials against Unnotched Tension/Compression (UNT/C) and Open Hole Tension/Compression (OHT/C) data for the same material systems within the NCAMP database. The intention of the selected material systems is to show validation of the multiscale material models developed with the same methodology against material system combinations including different fiber / same matrix, and same fiber / different matrix.

STUDY ON THE IMPROVEMENT OF OXIDATIVE SCALE DUST COLLECTION ABILITY IN STEEL PROCESS

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Key words: Dust Collector, Oxidative Scale, Collecting Hood, Discrete Phase Model

Abstract. The purpose of this study is to remove the scales occurring in the steel sheet when manufacturing steel. The scale that occurs in all manufacturing processes will pollute the working environment and will have an absolute impact on the health of worker, thus requiring scale removal. Normally, removing the scale improves the performance of the dust collector, which is costly and not efficient. In order to analyze the behavior of the scale, Computational Fluid Dynamics was performed. Based on the CFD results, a dust hood was developed to capture the contaminants without improving the performance of the dust collector. Because the size of the scale is variable, ordinarily dust collector is not efficient, and a dust collecting hood with a different method of collecting dust according to the scale size was developed and the performance was doubled.

1 INTRODUCTION

Generation of fine dust is a big issue all over the world, and it is a serious problem especially in the East Asian region. Due to the generation of fine dusts, diseases such as respiratory diseases are caused, and inconvenience of living and social problems are caused. As a result, not only has public interest in environmental pollution increased, but also environmental pollution has been strengthened both domestically and internationally. [1, 2] Thus, many devices and techniques for removing pollutants emitted to the atmosphere are being developed, and improvement of efficiency is a major concern as compared with the existing methods.

In the steel process, an oxide scale layer is formed on the surface of the strip by annealing. After the coils are wound up, the strips are loosened in the next process and the scales that fall off the surface of the steel sheet contaminate the equipment and the large scales are crushed to the size of the fine dust level. These oxide scales tend to contaminate the plant and escape to the factory door or window frame to increase the fine dust concentration in the atmosphere. There is a need to reduce the level of air pollution by eliminating the oxidation scale that occurs in industrial processes, improve the work environment in the plant and protect the health of workers.

The dust collecting method for removing air pollutants can be roughly divided into four types as filtration type, centrifugal type, washing type, and electric dust collecting type. In this study, we developed a hood that can improve the dust collecting efficiency of 10 μm or less by focusing on collecting contaminants instead of dust collecting methods. Because the fine dust - sized pollutants are light and are influenced by the flow of air, the Coanda effect is used to control the air flow. By controlling the flow of air, it is possible to control the behavior of the particles and to guide the scattered fine dust to the hood. [3]

The hood was designed using the Coanda effect [4] in order to accelerate the flow of air and the flow direction and the flow rate of air could be increased without any additional device. For this purpose, the hood design variables were determined and the optimal values were derived by determining the influence of each variable through the computational flow analysis. In order to simulate the actual flow of the scale particles, the behavior of the scales was investigated using the DPM(Discrete Phase Model) technique. [5]

2. PROBLEM DEFINITION

2.1 Analytical Model

The tension bridle roll which gives tension to the iron plate and the deflector roll which changes the direction use mainly similar size to maintain the equipment smoothly. The oxidized scale formed on the surface of the steel sheet after heat treatment is mainly in the hot-rolled steel sheet which is a hot-rolled steel sheet [6], and its thickness is more than about 2.0 mmt.

Figure 1 shows the flow field for analyzing the behavior of micro-dust generation schematics and the behavior of oxidation scales. It is the most common type of line that can be seen in actual steel process. In this line, the oxidized scale layer formed on the surface of the steel plate is scattered while passing through the curved path of the steel plate, which adversely affects the surrounding environment pollution, equipment aging and health of workers. The red dotted line represents the behavior of fine dust scales detached from the steel sheet surface, and the blue box represents the area of the analytical flow field of interest in this study.

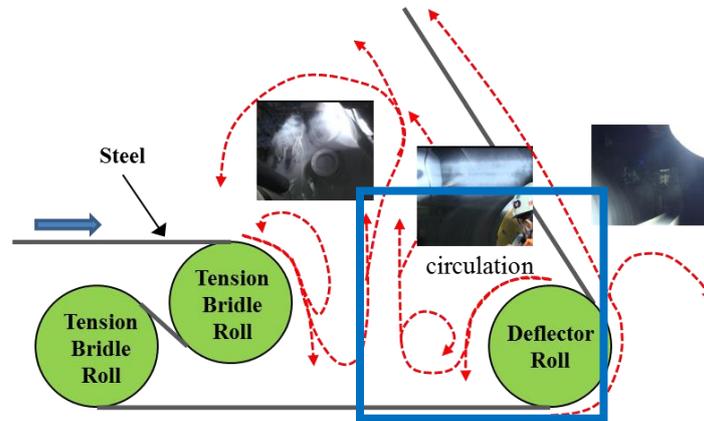


Figure 1 Process Schematic and Analytical Domain

The steel plate move in the direction from the lower part of the deflector roll to the upper left corner. The steel plate is bent in the tension bridle roll and the oxidized scales are dropped on the steel plate or floor. Due to this repeated situation, the scale is broken down and becomes smaller than the fine dust size, rising up to the upper part due to the flow of air due to the driving of the peripheral equipment.

For the analysis of the particle behavior on the flow field (blue line box) shown in Fig. 1, the lattice system is shown in Fig. 2 and nozzles with Coanda effect are installed on the upper and lower sides to remove fine dust scale. The air injected through the upper nozzle increase the air flow including the fine dust scale into the inside of the cover. The lower nozzle is also designed to capture the fine dust scale by increasing the air flow to the hood inlet while blocking the scale circulating on the roll.

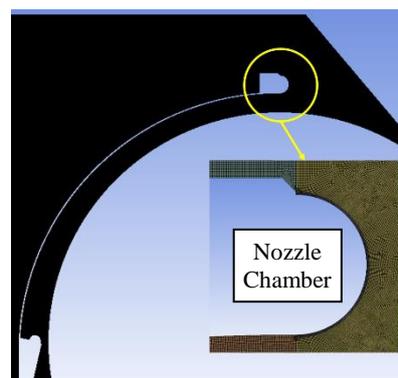


Figure 2 Mesh system

In order to understand the lattice dependence of the numerical solution, the number of

lattices was determined by comparing the numerical solutions according to the number of lattices and the number of lattices used in this numerical calculation was about 1.5 millions. Especially, in order to verify the Coanda effect that can maximize the air flow around the nozzle, a large number of meshes are formed on the solid surface at the bottom of the nozzle.

2.2 Limitations of Floating Size

In the process, there is much unpredictable turbulence due to the operation of equipment, the closing of factory doors, and the difference in temperature in the plant. However, the size of the scale floating in a static state can be known based on the equation of motion.

The forces received by the particles in the atmosphere are gravity by mass, buoyancy by the fluid, and surface resistance against the flow direction of the fluid. The working force and the definition of each force are shown in Fig. 3.

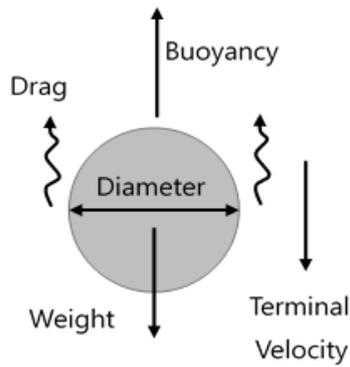


Figure 3 Forces acting on floating particle

The flow field in which the particles float can be assumed to be a creeping flow in which a very small flow is generated due to the driving of the plant. In the creeping flow field, the relation of all forces to the sphere is expressed as in Eq. (1), and the drag force in the flow field when Reynolds Number is less than 1 is expressed by Eq. (2) by the well-known Stoke's law.

$$F = m \frac{du}{dt} = F_w - F_b - F_d = mg - \frac{m\rho_a g}{\rho_s} - C_D A \frac{1}{2} \rho_a u_0^2$$

$$\text{here, } C_D = \frac{24}{\text{Re}} \tag{1}$$

$$F_d = 3\pi\mu u_0 D \tag{2}$$

Here, m is mass, g is gravitational acceleration, ρ_a is air density, ρ_s is density of scale, C_D is drag coefficient, μ is air viscosity, and Re is Reynolds number.

From these equations, drag force increases with increasing velocity of the particles falling in the fluid under gravity. Acceleration decreases with time, approaching zero and reaching a constant speed. This is called the terminal velocity. The terminal velocity of rounded particles is Eq. (3) with assuming that $du / dt = 0$ in Eq. (1).

$$u_t = \sqrt{\frac{4gD(\rho_s - \rho_a)}{3C_D\rho_a}} = \frac{gD^2(\rho_s - \rho_a)}{18\mu} \quad (3)$$

From this equation, the size of the particles reaching the termination speed can be expressed as Eq. (4).

$$D = \sqrt[3]{\frac{18Re\mu^2}{g\rho_a(\rho_s - \rho_a)}} = \frac{18\mu u_t}{g(\rho_s - \rho_a)} \quad (4)$$

From this, it can be seen that the size of the scale that floats without sinking in a static state is $0.23\mu\text{m}$ or less. However, in practice, the size of the scale that is floating due to the driving of the equipment and the surrounding of the door is larger than $0.23\mu\text{m}$. In this study, the behavior of particles with a fine particle size of $10\mu\text{m}$ is analyzed by controlling the air flow.

2. 3 Analysis of flow field

As shown in the analysis model in Section 2.1, numerical computation of fluid flow was performed assuming a 2 – dimensional since the roll is uniform in the longitudinal direction. The standard k- ϵ (SKE) turbulence model [7] was used to obtain numerical results of the flow field. The SKE model is known as the most used engineering turbulence model in the industry and has robust and reasonable accuracy. Compressibility, and buoyancy. The continuity equation, the momentum equation and the SKE transfer equation are shown in Eq. (5).

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) &= 0 \\ \frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) &= -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] + \frac{\partial}{\partial x_j}(-\rho \overline{u'_i u'_j}) \end{aligned} \quad (5)$$

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$$\begin{aligned}\frac{D(\rho k)}{Dt} &= \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \varepsilon \\ \frac{D(\rho \varepsilon)}{Dt} &= \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} G_k - \rho C_{\varepsilon 2} \frac{\varepsilon^2}{k} \\ C_\mu &= 0.09, \quad C_{\varepsilon 1} = 1.44, \quad C_{\varepsilon 2} = 1.92, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3\end{aligned}\tag{5}$$

Here, the ε - equation must use the wall function because it contains terms that are not computed from the wall. Generally, the effect is small for flows with large streamline curvature and large pressure gradient. In applying the general wall law, the momentum boundary condition is based on Launder-Spaulding law-of-the-wall and is shown in Eq. (6). A similar wall function was applied to energy.

$$U^* = \begin{cases} y^* & \text{for } y^* < y_v^* \\ \frac{1}{k} \ln(Ey^*) & \text{for } y^* > y_v^* \end{cases}, \quad U^* = \frac{U_p C_\mu^{1/4} k_p^{1/2}}{U_\tau^2}, \quad y^* = \frac{\rho C_\mu^{1/4} k_p^{1/2} y_p}{\mu}\tag{6}$$

2.4 Method of analyzing particle behavior

The DPM (Discrete Phase Model) technique was used to analyze the behavior of the fine dust scale in the flow field. The Lagrangian method was used to calculate the particle trajectory. The effect of the turbulence on the particles was the most common Stochastic tracking model. The above calculation was performed using FLUENT 17.2, the commercial CFD code. Additional minor features utilized default values given in commercial code.

2.5 Calculation Condition

The flow field is at atmospheric pressure and the rotation of the roll is 420 rpm in the counter clock wise direction and the linear velocity of the steel plate is 260 mpm. The scattered fine dust scale is composed of steel having a size of 0.1 ~ 10 μm and a rosin-rammler is applied to the diameter distribution. The flow rate was given as 10^{-20} kg / s. The specific gravity of the scale is 7.8 g / mm^3 , the density of air is 1.25 kg / m^3 , and the viscosity of air is 18×10^{-5} kg / m.s. The velocity at the top and bottom nozzles is given as 10.0 m / s.

2.6 Design parameters

In this study, the major parameters were set up for design to maximize collection efficiency. These design parameters are shown in Fig. 4. The parameters are the gap (S) of the nozzle tip injecting air, the nozzle bottom plate radius (R), the nozzle injection velocity (V) and the distance (H) from the roll.

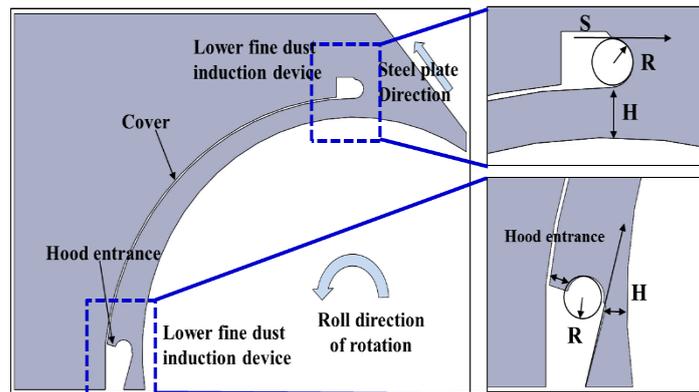


Figure 4 Design parameters

3. RESULTS AND DISCUSSION

3.1 Flow Characteristics

The flow characteristics of fine particle size scale particles in the flow field were investigated and the behavior and the collection efficiency of the particles when the particles were introduced into the calculated flow field were analyzed. The velocity and pressure distribution of the previous flow field is shown in Fig. 5.

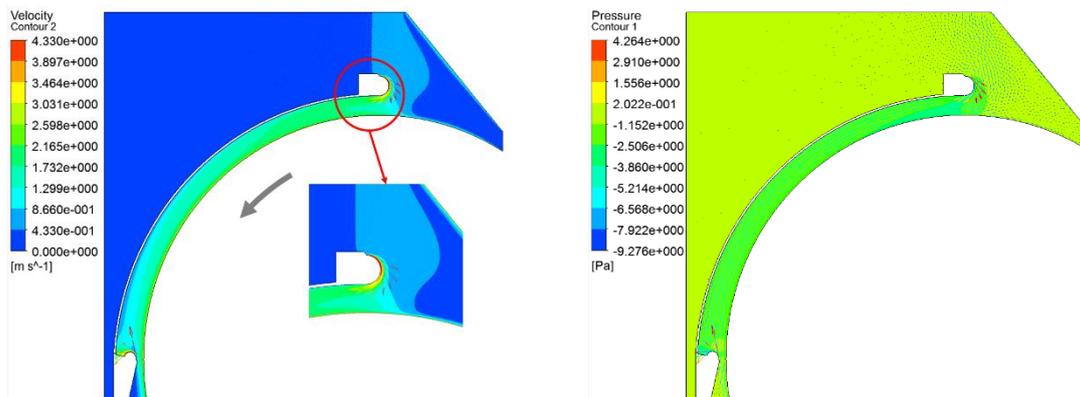


Figure 5 Contours of Velocity and Pressure

In this study, we focused on the nozzle which can induce the surrounding air and increase the flow rate, and it is confirmed that the flow field using this can realize the Coanda effect. By forming the curved surface of the lower part of the nozzle, the Coanda effect was obtained, and based on this, the design was established. The Coanda effect of air injected from the nozzle is shown in Fig. 6.

3.2 Effect of parameters

In this study, we analyzed the influence of major variables on design to maximize collection efficiency. It was found that there was no difference in the effect of the gap (S) of the nozzle tip injecting air and the nozzle bottom plate radius (R) was not significant. The faster the nozzle injection speed (V) was, the more favorable the effect was, but the effect was not clear. The Coanda effect, which changes the direction of flow along the lower curved surface, attracts more of the surrounding air, which means that it has a greater effect than the jet speed of the nozzle. However, the closer the flow plate height H is to the roll, the more effective it is to maximize the flow rate of the ambient air flow by the nozzle

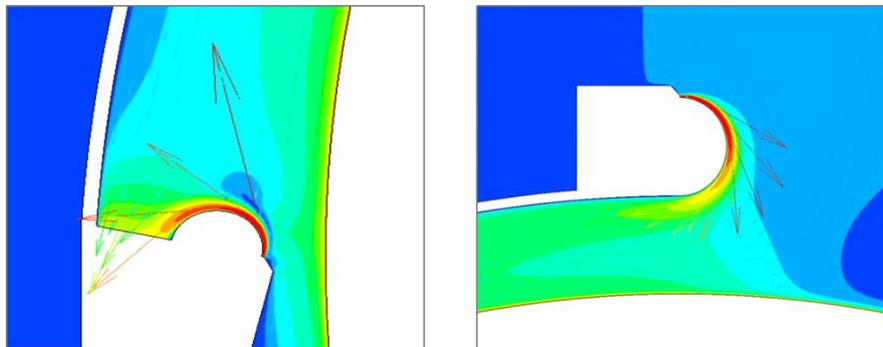


Figure 6 Coanda effect on the nozzle tip

4. CONCLUSION

Globally, especially in the East Asian region, the development of fine dust removal technology is ongoing to escape the threat of fine dust. In this study, we have developed a dust collecting system using numerical method in order to remove oxide scale of fine dust size floating off steel surface during steel manufacturing process. The principle of attracting the air flow and collecting the fine dust is applied to the fine dust scale of less than $10\mu\text{m}$ size which is influenced by the air flow. Nozzles were developed to utilize the Coanda effect to

induce airflow, thereby increasing ambient airflow. The influence of various design variables on the nozzle was analyzed and it was confirmed that the main factor, the nearby surface of the nozzle and the height of the flow plate in the roll.

In order to confirm the improvement of the dust collection efficiency, the dust concentration in the factory was measured and the standard of the Clean Air Conservation Act was achieved. The concentration of fine dust in the plant was 74%, lower than the legal standard, and the dust collection efficiency was doubled. This study will be helpful for the design of the dust collector in the future by designing the hood to capture the oxide scale of fine dust size.

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GPU Acceleration of Topology Optimization Methods

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ABSTRACT

In topology optimization methods it is well known that the relatively straightforward finite element calculations for the cost and constraint function values and their sensitivities remain major high performance computing bottlenecks. Indeed, the iterative nature of topology optimization necessitates solving the finite element problem as quickly as possible since each iteration requires one or more finite element simulations. At the same time, we would like to obtain higher fidelity designs and therefore we need to work on highly refined meshes which further increases the computational burden. To mitigate computational cost, we investigate the use of Graphics Processing Units (GPUs). Several strategies are examined to reduce the finite element runtime over cube-like topology optimization design domains in excess of 10 million elements. We use matrix-free methods on the GPU to solve larger problems and increase the effective memory bandwidth for sparse matrix-vector (SpMV) operations. Microkernel optimizations are invoked to optimize GPU kernel performance at both small and large scales. Data movement and the use of GPU clusters are also examined. Lastly, we examine the effect of matrix-free Jacobi and geometric multigrid preconditioners. Topology optimization examples demonstrate the collective effectiveness of these different strategies on cube-like design domains that incorporate adaptive meshing.

Developments on Sub-Grid Scale Modeling of Failure Mechanisms for Flood Control Systems in a Hydrodynamic Storm Surge Model

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ABSTRACT

Risk-informed decision making plays a critical role in mitigation of loss of life and assets during catastrophic events. This role is emphasized in coastal regions, which are susceptible to storm surge. Many factors, such as proximity to coastline and resilience of structures, directly influence the probable degree of risk posed to coastal regions by storm surge, though perhaps the most relevant and poorly understood factor is the ability of flood control systems to withstand forces attributed to storm surge and to protect coastal regions from inundation. Obtaining a proper understanding of this ability requires a multiphysics approach to modeling due to the intricate nature of the fluid-structure interactions involved during storm surge. Current available models are limited in their scope to provide information on this subject, e.g. current fragility based models frequently do not consider causal relationships and temporal correlations among multiple failure modes, and failure assessment often neglects the time evolution of processes leading to failure. We present on development of an adaptive-resolution storm surge model that responds to the changing state of flood control systems, designed to assist in overcoming of the aforementioned shortfalls. The storm surge model resolves failure mechanisms of flood control systems (e.g., wave run-up/overtopping, overflow, piping, sliding) as sub-grid scale processes. Results from the storm surge model are interfaced with geotechnical models in order to ensure the accuracy of the subgrid scale approaches. This presentation focuses on recent developments in resolving these failure mechanisms within a discontinuous Galerkin, shallow water equations based storm surge model (DG-SWEM [1]). Future goals include derivation of multi-dimensional time-dependent fragility models to be integrated with the storm surge model and ultimately lead to more informed decisions about catastrophic risk and infrastructure failure. [1] Dawson, C., Kubatko, E.J., Westerink, J.J., Trahana C., Mirabito, C., Michoskia C., Panda, N., Discontinuous Galerkin methods for modeling hurricane storm surge, *Advances in Water Resources*, 34, pp. 1165{1176, 2011.

A Symmetric Face-on-Face Contact Method for Implicit Nonlinear Solid Mechanics

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ABSTRACT

The implicit solution to contact problems in nonlinear solid mechanics poses many challenges. The discretization of the contact interface, form of the kinematic constraint, selection of a pressure basis, and the constraint enforcement method risk possible locking, contact force chatter in the presence of sliding, instability, non-physical or non-unique solutions, and equilibrium failure. This work seeks to address these issues whereby a symmetric face-on-face contact formulation is introduced for frictionless contact using three-dimensional, trilinear hexahedral finite elements. A set of opposing contact face-pairs is defined where a median plane methodology is used to construct local face-pair overlaps. These overlaps represent contact patches, the union of which constitutes the contact surface discretization. An up-to linear pressure basis is defined over each contact patch, whose active degrees of freedom are determined in a way that eliminates over-constraint. The resulting linear monomials are used as test functions for an integral form kinematic gap constraint. The gap constraints are enforced using a subcycle procedure that enforces both active and in-active constraints. This method is shown to handle complex contact interfaces in the presence of geometric and material nonlinearity resulting in physical and kinematically admissible solutions.

Treatment of Large Deformation Contact using VEM

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ABSTRACT

In most classical contact computations nodes are projected on parametrized surfaces where then contact constraints are enforced in tangential and normal direction to differentiate between stick and slip state. As an alternative, contact can be computed just by coupling of the nodes and assuming stick. The sliding case is then considered afterwards by letting the projected node follow a friction cone defined by normal and tangential tractions of Coulomb's law. This technique was applied to node-to-segment contact discretizations first in [1]. With the introduction of the Virtual Element Method [2] another possibility to formulate contact discretizations is offered by the flexibility of VEM to insert new nodes. Hence it will be possible to set up node-to-node formulations, even for sliding and for finite deformations. The approach is based on freely adding contact nodes to the original mesh [3] by this one easily overcomes differences in mesh size and surface interpolation. In combination with the moving cone description the VEM contact offers a simple formulation for surfaces in sliding contact. Contrary to classical node-to-node contact sliding movement is possible by adjusting the position of the contact nodes in the mesh according to the friction state. In the presentation a short introduction to the virtual element method for large deformations [4] is presented which will be the basis of the formulation. The projection algorithm for node-to-node contact is discussed next. Then the presentation will focus on the algorithmic scheme for the node adjustment due to the sliding motion. The resulting formulation will be compared to classical contact treatments with respect to performance and accuracy.

Pairwise Hydrodynamic Interactions of Vesicles in Applied Electric Fields

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ABSTRACT

The electrohydrodynamics (EHD) of vesicle suspensions is characterized by studying their pairwise interactions in applied DC electric fields in two dimensions. A boundary integral equation (BIE) based formulation for vesicle EHD is introduced, followed by a solution scheme based on Stokes and Laplace potential theory. In the dilute limit, the rheology of the suspension is shown to vary nonlinearly with the electric conductivity ratio of the interior and exterior fluids. We demonstrate our capability of simulating EHD phenomena including one vesicle deformation, pairwise interaction, and multiple vesicle interactions.

A Stable and Convergent Lagrangian Particle Method for Large Strain and Material Failure Analyses in Manufacturing Processes

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ABSTRACT

In this paper, we present a new Lagrangian particle method for the simulation of manufacturing processes involving large strain and material failure. The starting point is to introduce some penalty terms as a means of circumventing the onerous zero-energy deformation in the Lagrangian particle method. The penalty terms are derived from the approximate strain vector by the combination of a constant and a strain derivative leading to a dual stress points algorithm for stabilization. The resultant stabilized Lagrangian particle formulation is a non-residual type which renders no artificial control parameters in stabilization procedure. Subsequently, the stabilized formulation is supplemented by an adaptive anisotropic Lagrangian kernel and a bond-based material failure criterion to sufficiently prevent the tension instability and excessive straining problems. Several numerical examples are utilized to examine the effectiveness and accuracy of present method for modeling large strain and material failure in manufacturing processes.

Several Key Concerns in the Development of Numerical Tank

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ABSTRACT

CFD application is one of the most impressive progressions in the research on ship hydrodynamics. It is now becoming a powerful tool and involved intensively in the procedure of ship design. Numerical tank is a common vision for all the marine CFD man, which is presented to reinforce or even substitute model test in real tank. With the rapid development of CFD application and correlative technologies, "numerical tank" is now a hotspot in the research field of marine hydrodynamics. Nowadays, many attentions and efforts are paid on numerical tank. However, some key concerns about numerical tank are unclear. Such as, what is numerical tank? What are the technical contents and characters of numerical tank? How to ensure the accuracy of the result from numerical tank? These concerns are critical to the development of numerical tank. The research team of China Ship Scientific Research Center has made many efforts and is making continuing efforts now on the development of numerical tank. In this paper, the definition, technical contents and characters of numerical tank will be given out and discussed based on our research and practice. In our opinion, numerical tank is an application system based on reliable CFD technology which can provide service to the client as real tank does. The core value of numerical tank is practical application. The way of developing numerical tank can be knowledge packaged after attribute subdivision and can achieve the purpose of "developed by expert and used by common client". The differences between numerical tank and CFD in several aspects will also be analyzed, the two families of key technologies in the research of CFD and development of numerical tank will be presented and discussed. As an example, the key technology of confidence level assessment for the results of ship model resistance from numerical will be introduced in detail. The methodology of confidence level assessment is based on the procedure of "uncertainty analysis, validation of optimal solution, validation by big sample data". In which the uncertainty analysis is based on orthogonal design and variance analysis methods and statistic inference theory, the validation of optimal solution is based on effect analysis in orthogonal design and principle of minimum deviation; the virtual test method is validated by statistical analysis of comparison with a large numbers of model test data.

Properties and Functions of Soft Materials in a Honeybee Tongue

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ABSTRACT

Many biological structures can perform highly-dexterous actions by using soft materials. To achieve high feeding efficiency but low energy expenditure during nectar feeding, the glossal surface of a honeybee undergoes shape changes, in which tongue hairs erect together with segment elongation in a drinking cycle. We discovered a transmission link embedded in the glossa from postmortem examination connected by intersegmental membranes which consists of chitin and protein. Compliance of soft materials provides more possibilities for its high deformation and kinematic synchronicity between tongue body and hairs. We measured the mechanical properties of this soft material and modeled the tongue structure as a compliant mechanism. It is validated that soft material contributes to not only a higher flexibility of the honeybee's tongue, but a higher capacity of elastic potential energy transfer rate. This work may arouse new prospects for conceptual design of micro-mechanical systems equipped with bio-inspired soft connections.

A Probabilistic Mean-Field-Homogenization Approach Applied to Study Unidirectional Composite Structures

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ABSTRACT

In order to account for micro-structural geometrical and material properties in an accurate way, homogenization-based multiscale approaches have been widely developed. However, most of the approaches assume the existence of a statistically Representative Volume Element (RVE), which does not always exist for composite materials due to the existing micro-structural uncertainties, in particular when studying the onset of failure. In this work we develop a stochastic multi-scale approach for unidirectional composite materials in order to predict scatter at the structural behavior. First Stochastic Volume Elements (SVE) [1] are built from experimental measurements. Toward this end, statistical functions of the fibers features are extracted from SEM images to generate statistical functions of the micro-structure. The dependent variables are then represented using the copula framework, allowing generating micro-structures, which respect the statistical information, using a fiber additive process [1]. Probabilistic meso-scale stochastic behaviors are then extracted from direct numerical simulations of the generated SVEs, defining random fields of homogenized properties [2]. Finally, in order to provide an efficient way of generating meso-scale random fields, while keeping information, such as stress/strain fields, at the micro-scale during the resolution of macro-scale stochastic finite element, a probabilistic Mean-Field-Homogenization (MFH) method is developed. To this end, the phase parameters of the MFH are seen as random fields defined by inverse stochastic identification of the stochastic homogenized properties obtained through the stochastic direct simulations of the SVEs. As a result, non-deterministic macro-scale behaviors can be studied while having access to the micro-scale different phases stress-strain evolution, allowing to predict composite failure in a probabilistic way. [1] M. Ostoja-Starzewski, X. Wang, Stochastic finite elements as a bridge between random material microstructure and global response, *Computer Methods in Applied Mechanics and Engineering* 168 (14) (1999) 35 - 49 [2] L. Wu, C.N. Chung, Z. Major, L. Adam, L. Noels. From SEM images to elastic responses: a stochastic multiscale analysis of UD fiber reinforced composites. Submitted to *Composite Structures* [3] V. Lucas, J.-C. Golinval, S. Paquay, V.-D. Nguyen, L. Noels, L. Wu, A stochastic computational multiscale approach; Application to MEMS resonators, *Computer Methods in Applied Mechanics and Engineering* 294 (2015) 141 - 167

Investigating Cross-Species Scaling for Traumatic Brain Injuries Using Finite Element Analysis

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ABSTRACT

Animal injury models are widely used as surrogates for humans for the study of the mechanisms and the biomechanical thresholds of traumatic brain injury (TBI). However, one important question exists for translating animal responses to humans: how does the impact conditions and resulting biological response scale across species of various brain sizes and shapes. Simplified scaling methods based on structural similitude have guided the interpretation of animal data in the context of humans, but these methods are unvalidated and are criticized because they do not consider the differences in brain anatomy and shape of each species. Investigations using finite element (FE) models of brains from multiple species can address some of the limitations that exist with TBI scaling methods. Previously developed human (Mao et al. 2013) and non-human primate (Antona-Makoshi. 2016) FE brain models were modified to harmonize various modeling methods and anatomical features such as axonal tract information and brain tissue constitutive models. Where possible, the new brain models were validated against existing brain deformation test data and demonstrated good biofidelity. A parametric study was performed for each brain model simulated under a range of rotational head kinematics consistent with injury model data presented in the literature. Tissue-level injury metrics were recorded for each simulation, and model responses were compared across species under the assumption that comparable metrics result in comparable clinical outcome. Traditional scaling methods were evaluated against the predicted FE model data output. Relationships between tissue-level metrics, including maximum principal strain (MPS), the cumulative strain damage measure (CSDM) and maximum axonal strain (MAS), and applied head kinematics were formulated in angular acceleration-angular velocity space in a manner similar to Gabler et al. (2017). The metrics predicted by the FE models were different compared with those measured using traditional kinematic scaling methods. Compared with traditional scaling methods, using FE models to study cross-species TBI mechanics enabled the consideration for the differences between species in brain physical morphology, anatomy, tissue properties. Further efforts will focus on investigating the correlation between strain responses and pathology results. Overall, this study provided an improved method for scaling animal experiments and tissue injury metrics to humans. Reference Antona-Makoshi, J. (2016). PhD Thesis, Chalmers. Gabler, L. F. et al. (2017). J Biomech Eng. Mao H, et al. (2013). J Biomech Eng.135(11):111002.

Tightly Coupled, Partitioned Fluid-Structure Interaction Modeling Framework for Naval Applications: The Impact of Slamming Loads on High Speed Watercraft

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ABSTRACT

The current presentation reports on the effort to couple of our in-house computational structural dynamics software (CU-BEN) with a widely used computational fluid dynamics C++ API (OpenFOAM), in order to study the very challenging Fluid-Structure Interaction (FSI) problem known as “slamming.” Slamming occurs when shell surfaces, comprising the outer hull plating on high speed watercraft, impact the liquid phase in a way that has the shell normal nearly orthogonal to the free surface. Due to the relative densities between the liquid and solid phases, two-way coupling is required to handle the so-called “added mass effects.” Slamming loads cause very high strain rates and nonlinear responses within the solid domain; thus these aspects are considered in the CSD modeling. Additionally, the flat configuration of the structure, relative to the liquid free surface, presents significant opportunity for air to become trapped and compressed at the interface; thus a gas phase is admitted within our modeling. Given the tiny spatiotemporal scales in play within this particular phenomenology, experimental work has been limited; thus hampering the development of robust and accurate theoretical constructs. The present research aims at creating a kind of “FSI microscope”; to better investigate the context of slamming. Early applications of this simulation tool will inform experimental work of our collaborators; the results of which will subsequently be used as part of a formal model validation effort for the FSI simulation capability underdevelopment. The subsequently validated model will then be used, in conjunction with the experiments of our collaborators, to arrive at improved engineering theories describing slamming phenomena.

Turbulent-Turbulent Spot as the Inner-Layer Coherent Structure of Turbulent Boundary Layer

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ABSTRACT

There has been a general consensus that the dynamically important coherent structures inside the viscous sublayer and buffer layer of wall-bounded turbulent flows are low-momentum streaks and randomly distributed quasi-streamwise vortices. While this consensus is supported by direct numerical simulation (DNS) data for internal flows such as the fully-developed turbulent channel flow, there is actually very little supporting evidence coming from the external boundary layer flow. On the contrary, wind-tunnel experimental visualization in the 1970s by R.E. Falco on the viscous sublayer of the zero-pressure-gradient flat-plate boundary layer show that the viscous sublayer is dominated by pockets. Unfortunately, this important piece of evidence on viscous sublayer pockets has often been overlooked and ignored in the past because it contradicts with the mainstream idea of quasi-streamwise vortices and streaks. From our accurate, physically-realistic, spatially-developing DNS on the zero-pressure-gradient flat-plate boundary layer, we discovered that the inner layer of the turbulent boundary layer is dominated by turbulent-turbulent spots. These are defined as dense concentrations of small-scale vortices with high swirling strength originating from hairpin packets. Although structurally quite similar to the transitional-turbulent spots, these turbulent-turbulent spots are generated locally in the fully-turbulent environment, and they are persistent with a systematic variation of detection threshold level. The turbulent-turbulent spots exert indentation, segmentation and termination on the viscous sublayer streaks, thus creating pockets. The turbulent-turbulent spots coincide with local concentrations of high levels of Reynolds shear stress, enstrophy and temperature fluctuations, hence are dynamically important for turbulent transport processes. The sublayer streaks seem to be passive and are often simply the rims of the indentation pockets arising from the turbulent-turbulent spots. This work provides the first DNS confirmation on the existence of viscous sublayer pockets. Inside the viscous sublayer and the buffer layer, the dynamically important coherent structures of the boundary layer are turbulent-turbulent spots rather than quasi-streamwise vortices and streaks. The present boundary layer develops from a laminar Blasius solution at momentum-thickness Reynolds number 80 beneath a freestream decaying isotropic turbulence whose initial intensity is 3 percent. The boundary layer goes through a process of bypass transition in the narrow sense, reaching fully-turbulent state with an exit momentum-thickness Reynolds number of 3000. The accuracy of the DNS results is thoroughly validated against an array of existing experimental, numerical and theoretical data.

Wider Strain-rate Dependent Damage Constitutive Model and Application in Penetration Simulation for PBX explosives

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ABSTRACT

Polymer-bonded explosives (PBXs) are a family of composite materials formulated with polymeric binder system and hard phase explosive crystals. Damage of PBXs caused by external stimulus influences not only the mechanical properties, but also the sensitivity, combustion and even detonation behavior of energetic materials because cracks, pores or debonding can act as fast reaction channels. The characteristic damage modes present in PBXs include intragranular voids, crystal fractures, and interfacial debonding. A three-dimensional viscoelastic model taking into account above three damage mechanisms has been developed to describe the mechanical response at wide strain rate range (10^{-3} ~ 10^4 s⁻¹). We can obtain the respective contributions of different damages to mechanical behavior, corresponding to different mechanical stimulus from quasi-static loading to high-strain-rate dynamic conditions. uniaxial compression tests were performed with the loading speed 5 mm/min and 1.0mm/min from 22°C to 75°C on some PBX. The Abaqus user subroutines UMAT and VUMAT were formulated based on the damage-coupled viscoelastic constitutive theory. Experimental quasi-static and dynamic compression data at some loading rates and different temperatures are used to validate the model and calibrate the constitutive parameters. The comparisons between simulated and experimental results under pure compressions loading show good agreements. When the projectile filled with explosive charge penetrates the target plate, the charge undergoes complex stress history, including the shock wave loading through the shell, and high inertial force, as well as loop loading and unloading due to shock wave reflection. The dynamic damage viscoelastic model is used to simulating the explosive charge filled in steel projectile in penetrating concrete target. Dissipation heat from plastic work, volume compression work and viscous flow work were included in the model. The penetration simulation showed that the compression stress wave is input into the explosive charge from the head and turn into tension reflected wave at the tail. By analyzing the damage distribution, the temperature distribution and the variations of plastic work and internal energy at different segment, the condition under which that explosive charge is prone to ignite can be predicted. Debonding damage tends to occur at the boundary elements near the shell inside surface. With the penetration proceeds, debonding damage diffuses from boarder area to the centerline area. The simulated results provide relevance between mechanical damage and ignition sensitivity of explosive charge, which are important for projectile structure design and safety evaluation.

Industrial Applications of the Smoothed Particle Galerkin (SPG) Method in Ductile Failure Analysis

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ABSTRACT

Abstract This work presents the industrial applications of the Smoothed Particle Galerkin (SPG) method [1, 2] in LS-DYNA® in ductile failure analysis. The SPG method is a new generation meshfree method developed for modeling semi-brittle and ductile material failure [3-5]. Different from the conventional finite element method (FEM) where the element erosion technique is utilized to mimic the material separation, the SPG method introduces a bond-based material failure mechanism to reproduce the strong discontinuity in displacement field without sacrificing the conservation properties of the system equations. The mathematical and numerical analyses have suggested that the SPG scheme is stable and convergent in modeling material failure processes. Currently, one of the major applications of the SPG method is the simulation of destructive manufacturing processes such as metal cutting, drilling, machining and shearing, and jointing processes such as riveting and screwing. The SPG method can also be applied to model the material failure in high velocity impact penetration problems. To show the effectiveness of the SPG method in analyzing ductile failure phenomena, industrial processes such as metal machining and high velocity impact penetration are modeled in this research. To further investigate the performance of the SPG method in those applications, parametric and convergence studies including the effects of bond failure criteria, nodal support size and domain discretization will be elaborated as well. Reference: [1] Wu CT, Koishi M, Hu W. A displacement smoothing induced strain gradient stabilization for the meshfree Galerkin nodal integration method. *Comput. Mech.* 56, 19-37, 2015. [2] Wu CT, Chi SW, Koishi M, Wu Y. Strain gradient stabilization with dual stress points for the meshfree nodal integration method in inelastic analysis. *Int. J. Numer. Methods Engrg.* 107, 3-30, 2016. [3] Wu CT, Bui TQ, Wu Y, Luo TL, Wang M, Liao CC, Chen PY, Lai YS. Numerical and experimental validation of a particle Galerkin method for metal grinding simulation. *Comput. Mech.* <https://doi.org/10.1007/s00466-017-1456-6>, 2017. [4] Wu CT, Wu Y, Crawford JE, Magallanes JM. Three-dimensional concrete impact and penetration simulations using the smoothed particle Galerkin method. *Int. J. Impact Engrg.* 106, 1-17, 2017. [5] Wu Y, Wu CT. Simulation of impact penetration and perforation of metal targets using the smoothed particle Galerkin method. In publication, *J. Engrg. Mech.* 2017.

Dynamic Buckling of Variable Angle Tow Composite Panels

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ABSTRACT

Recently, variable angle tow (VAT) composites that offer an extended point wise stiffness tailoring capability for structural designers have attracted significant research interests. In this paper, the dynamic buckling behaviour of geometrically imperfect variable angle tow composite plates under longitudinal compressive pulse loading is studied. From the design point of view, even if a plate is capable of withstanding a particular amount of static in-plane compressive loading before buckling it may buckle earlier with a dynamic load of lower magnitude. The nature and duration of the dynamic load has a significant effect on the buckling behaviour. This work aims to explore the benign features offered by variable angle tow composites to enhance the dynamic buckling performance of rectangular plates. An efficient and robust semi-analytical modelling based on a mixed Hellinger-Reissner variational principle is developed to solve the dynamic buckling problem for VAT composite plates. Geometric imperfection, the nonlinearity induced by large deflections, and wave propagation effects given by in-plane inertia properties, are included in this newly developed dynamic buckling model. Both force and displacement controlled pulses loading are considered. Appropriate criteria are employed to assess the dynamic buckling behaviour under various loading types. Finite element model for the dynamic buckling analysis of VAT plates is also developed using the commercial package ABAQUS for the validation of numerical results given by the present model. The dynamic buckling behaviour characteristics of VAT plates subject to different in-plane boundary conditions are determined and analysed by studying their critical buckling loads and transverse deflection responses. Furthermore, a parametric study on the dynamic buckling response of VAT plates with linear variation of fibre angle is performed. The benefits of applying the VAT laminates to improve the dynamic buckling performance of rectangular plates are clearly demonstrated through comparing with the results of straight-fibre laminates. [1] Z. Gürdal, B.F. Tatting and C. K. Wu "Variable stiffness composite panels: Effects of stiffness variation on the in-plane and buckling response". Composites Part A: Applied Science and Manufacturing, Vol. 39, No. 5, pp 911-922, 2008. [2] Z. Wu, P.M. Weaver, G. Raju, and B. C. Kim "Buckling analysis and optimisation of variable angle tow composite plates". Thin-Walled Structures, Vol 60, pp163-172, 2012. [3] B. Budiansky, and John W. Hutchinson. "Dynamic buckling of imperfection-sensitive structures." Applied Mechanics. Springer Berlin Heidelberg, 1966. 636-651.

A File-Based Storage Approach to a Public Turbulence Database System and Applications to a Transitional Developing Boundary Layer Dataset

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ABSTRACT

The Johns Hopkins Turbulence Databases (JHTDB, at <http://turbulence.pha.jhu.edu>) has been providing public access to several large DNS datasets through web services. In the previous version of JHTDB (Li et al., JoT, 2008; Kanov, thesis, 2015), the simulation data were converted and then ingested into SQL tables in SQL data servers. This ingestion process is complex and for 100 TB datasets may take months. This challenge has motivated the development of a new file-based data storage approach for JHTDB that enables easier and more streamlined setup of datasets. This approach is called FileDB; the databases are stored as files instead of SQL tables in the previous versions of JHTDB. As in the SQL-based system, in FileDB the simulation data are partitioned into data atoms of 8^3 . The atom is the fundamental unit of I/O operations. The size of the atom is chosen to balance the I/O time and disk seeking cost. The atom is indexed in z-order (also known as Morton order) for its good spatial locality. The converted data are then stored as binary files on data servers. For some datasets, the grid point number may not be a multiple of eight in one or more directions. In this case, the domain for which data are stored can be cut in that direction, or zero-padded. If the grid point numbers are not the same in all three directions, the atom z-indices can be discontinuous. In this case, a separate SQL table is created to store the atom z-indices that actually exist in the simulation domain. In this way, the JHTDB with FileDB can ingest more general simulation data, e.g. developing boundary layer (Lee and Zaki, APS/DFD, 2015). Three new datasets, a snapshot of isotropic turbulence on a 4096^3 grid, five snapshots of rotating stratified turbulence on a 4096^3 grid and a full time-history of a developing boundary layer flow over a smooth surface, are added to the JHTDB using fileDB. By avoiding the ingestion process, we have managed to achieve a massive speed up. For task parallelism when accessing these data on JHTDB, the data are distributed among nodes of the database cluster. The evaluation shows the performance of fileDB is as good as the previous SQL approach, with the added benefit of lower latency per request. Some sample results of analysis of geometric features of the turbulent/non-turbulent interface in the developing portion of the boundary layer will be presented.

An Application of State Space Method in Surface Instability Analysis for Graded Soft Materials

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ABSTRACT

Surface instability of film-substrate system has been analyzed intensively for many years. For graded layers with depth-wise variation in material properties, the analytical solution for critical condition of surface instability cannot be obtained in general, thus the numerical method, such as the finite element method, was commonly employed for such cases. In the current presentation, we suggest a state space method for analyzing surface instability of graded layers with material properties varying in the thickness direction. Based on the governing equations for the surface instability of graded elastic layers and graded hydrogel layers, by discretizing the material properties into piecewise constant functions with homogeneous sub-layers, a state space method was developed to solve the eigenvalue problem and predict the critical condition for onset of surface instability. For the graded elastic system, results were presented for bilayers and continuously graded elastic layers. The state space solutions for elastic bilayers are in close agreement with the analytical solution for thin film wrinkling within the limit of linear elasticity. Numerical solutions for continuously graded elastic layers were compared to finite element results in a previous study (Lee et al., 2008, *J. Mech. Phys. Solids* 56, pp. 858–868). For the hydrogel system, the state space solutions for homogeneous hydrogel layers and hydrogel bilayers were compared to the finite difference results and analytical solutions. While the finite difference method often requires a large number of nodes to achieve convergence, the state space method requires relatively fewer sub-layers for continuously graded layers. The results for linearly and exponentially graded hydrogel layers show that the critical swelling ratio and corresponding critical wavelength both depend on the gradient profile of the crosslink density. In addition, the surface instability of graded elastic cylinders was also examined by the state space method. The state space solutions for three typical examples were acquired and show to be in good agreement with the numerical results by the finite element method, including the analytical solution for a thin cylindrical shell. In particular, a transition of the critical buckling mode for a soft cylinder covered by a bilayer was illustrated clearly by the present method. In contrast to the finite element method and finite difference method, the state space method is a semi-analytical approach with good convenience and higher computational efficiency for arbitrarily graded materials, including layered structures.

Multiscale Modeling for Instability Phenomena of Long Fiber Reinforced Composite with A Double Scale Microscopic Model

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ABSTRACT

The fiber microbuckling in long fiber composites may lead to the compressive failure of the macrostructure. To study such a multiscale problem, direct simulation is limited due to the expensive computation cost and difficulties in selecting non-linear calculation paths because there exists a lot of bifurcation points around the useful one. This work is to propose an efficient multiscale model for accurately simulating and analyzing the instability phenomena of long fiber reinforced materials. The multi-level finite element method [1] (FE^2) is adopted to realize the real-time interaction between macro- and microscopic levels: the macroscopic constitutive law is calculated on the Representative Volume Element (RVE), and the microscopic deformation gradient is transferred from the associated macroscopic Gauss point. However, the total computation cost may be still very high because the RVE on each Gauss point of macroscopic model needs a sufficient fine mesh to simulate the microbuckling of long fibers. Thus, a Fourier related double scale microscopic model [2] is developed to transform the fast varying microscopic unknowns into a series of slowly varying unknowns which only requires remarkably reduced meshes. In addition, the new RVE model allows one to control non-linear calculation paths easily by choosing the wavelength of the buckled fiber. The developed non-linear multiscale model is solved by the Asymptotic Numerical Method [3] (ANM), which is less time consuming and more stable than other classical iterative methods. The established multiscale model yields accurate results with a significantly improved computational efficiency. Keywords: Fourier series, Long fiber reinforced composites, RVE, FE^2 method, Instability. References [1] S. Nezamabadi, J. Yvonnet, H. Zahrouni, M. Potier-Ferry, A multilevel computational strategy for handling microscopic and macroscopic instabilities, *Computer Methods in Applied Mechanics and Engineering*, 198, 2099-2110, 2009. [2] Y. Liu, K. Yu, H. Hu, S. Belouettar, M. Potier-Ferry, N. Damil, A new Fourier-related double scale analysis for instability phenomena in sandwich structures, *International Journal of Solids and Structures*, 49, 3077-3088, 2012. [3] B. Cochelin, N. Damil, M. Potier-Ferry, Asymptotic-numerical methods and Padé approximants for nonlinear elastic structures. *International Journal for Numerical Methods in Engineering*, 37, 1187-1213, 1994.

Negative Poisson's Ratio Design of the Cardiovascular Stent Using a Level Set-based Parameterization Method

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ABSTRACT

Abstract: Implanting stent is an important surgical way for treating a wide range of cardiovascular disease, but it will cause a physic injury for the vascular during the process, due to the variable shape of the vascular in the axial direction. So, the compliance of the stent is different in radial and axial directions. As for the former, the compliance should be minimized to support the vascular, while in another direction, the stent needs to comply the different shapes of the vascular as soon as possible. This paper presents a novel design work of the cardiovascular stent with a negative Poisson's ratio(NPR) to increase the compliance in the axial direction to reduce that damage. Moreover, the NPR stent is much shorter than the traditional one when ready for the implantation, no matter for self-expanding or balloon-expanding stent, which significantly increase the successful ratio of the operation. Although, there are many research studies on NPR design by using microstructure design method currently, this kind of metamaterials is hardly meeting the compliance requirements on the macro scale of the stent. So, this research proposes a new NPR design method. At first, the NPR structure will be obtained on the micro scale, and then it will transfer the microstructure to macrostructure by considering the working conditions in the vascular. During the microscale design, the macro compliance requirements will be considered in both directions to limit the structure of NPR, since the same NPR can have many different structures. In this paper, a level Set-based parameterization topology optimization method is used. It can obtain a structure with a clear boundary shape, which is an essential part of stent design because this research uses a micro scale design to get a macrostructure, and a small difference on the shape will lead to significant changes on the properties. Meanwhile, parameterization can control the boundary change very well. Finally, the new NPR stent structure will be tested by ANSYS. Keywords: Negative Poisson's ratio, stent, level set, parameterization, topology optimization

A Spectral Method to Study the Onset of Necking Instability for Dynamic Plane Strain

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ABSTRACT

During dynamic expansion of thin ductile metal cylinders, the deformation is first homogeneous. Then necking instabilities appear which generate local thinning, triggering plastic localization and finally the fragmentation of the structure. The present work aim is to provide new developments for the predictions of the fragment size and velocity. In order to study the onset of necking instability, linear stability analyses (LSA) are adopted to determine a critical wavelength which develops with the fastest growth rate. It has been shown that LSA can provide deep understandings of experimental results like the number of necks or their time of occurrence after some calibrations [1][2] However, the previous approaches suffer from some drawbacks. Indeed, based on a frozen coefficient theory, the model is salient when the time scale inherited from the development of the necking is smaller than the time scale of the background solution (homogeneous deformation without any imperfections). Such conditions are no more satisfied for stretching rate over 10000 per second. In the present talk, a new contribution is proposed. The time and space evolution of any perturbations is captured via a system of linearized equations. A Tau spectral method is adopted. Dynamic plane strain loading is investigated on a thin plate configuration, representative of a thin cylinder expansion. The material is incompressible. Its behavior is rigid viscoplastic, satisfying a J2 flow theory . As a result, different initial geometrical defects representative of material heterogeneities and forming defects have been considered. Their time and space evolution have been captured by the new method. It has been seen that while the perturbation evolution is highly depending on the shape of the defect in the early stage of the deformation process, their long term evolution is quite close to the one predicted by the classical LSA. We have checked that at least for strain rate lower than 1000 per second, the instantaneous growth rates predicted by the classical LSA and the new contribution are consistent. In a next step, larger strain rate loading will be investigated. In addition, to further validate the present approach, finite element simulations are planned. References: [1] Mercier and Molinari, Analysis of multiple necking in rings under rapid radial expansion, 2004, International Journal of Impact Engineering 30, 403-419 [2] Jouve, Étude analytique de l'instabilité plastique de striction pour une plaque sollicitée en traction biaxiale, 2010, École Polytechnique and Commissariat à l'Énergie Atomique, France

Topology Optimization of Quasi-brittle Composites for Fracture Resistance with Phase Field Modeling of Crack Propagation

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ABSTRACT

In this work, we propose a numerical framework for optimizing the fracture resistance of quasi-brittle composites through a modification of the topology of the inclusion phase. The phase field method to fracturing is adopted within a regularized description of discontinuities, allowing to take into account cracking in regular meshes, which is highly advantageous for topology optimization purpose. Extended bi-directional evolutionary structural optimization (BESO) method is employed and formulated to find the optimal distribution of inclusion phase, given a target volume fraction of inclusion and seeking a maximal fracture resistance. A computationally efficient adjoint sensitivity formulation is derived to account for the whole fracturing process, involving crack initiation, propagation and complete failure of the specimen. The effectiveness of developed framework is illustrated through a series of 2D and 3D benchmark tests. It has been shown that significant improvement of the fracture resistance of composites has been achieved for designs accounting for full failure when compared to conventional linear designs. Compared to previous studies in the literature on the subject, this work provides a much more efficient alternative for the design of high fracture resistant composites. There exist twofold merits of the developed design framework: on the one hand, the adoption of topology optimization provides uttermost design freedom, yielding higher fracture resistant designs; on the other hand, limited number of iterations is required for the design for the sake of using gradient information, which is of essential importance dealing with computationally demanding fracturing simulation.

Achieving Temperature Transferable Coarse-Graining of Polymers and Glass-Forming Materials via Energy Renormalization

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ABSTRACT

The bottom-up prediction of the properties of polymeric and glass-forming materials based on molecular dynamics simulation is a grand challenge in soft matter physics. Coarse-grained (CG) modeling is often employed to access greater spatiotemporal scales required for many applications. However, there is currently no temperature transferable and chemically specific coarse-graining method that allows for modeling of polymer dynamics over a wide temperature range. Here, we pragmatically address this issue by “correcting” for deviations in activation free energies that occur upon coarse-graining. In particular, we propose an energy-renormalization (ER) strategy to coarse-graining polymers based on relationships drawn from the Adam-Gibbs theory of glass formation, in conjunction with the localization model of relaxation. By testing different glass-forming materials ranging from fragile polymers to small molecules, we show that our ER approach can faithfully estimate the diffusive, segmental and glassy dynamics of the AA model over a large temperature range spanning from the Arrhenius melt to the non-equilibrium glassy states. Our proposed CG approach offers a promising strategy for developing thermodynamically consistent CG models with temperature transferability.

Exact Geometry Based Quasi-Conforming Analysis: Isogeometric Analysis Method with Quasi-Conforming Techniques

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ABSTRACT

Isogeometric analysis (IGA) is proposed by Prof. T.J.R. Hughes et al. as an alternative solution for computer aided engineering. In the past decade it has been developed into a powerful numerical method which has solid mathematical theory, excellent numerical efficiency, precision and versatile ability for engineering applications. The innovative idea to use splines as approximate functions for both geometry and unknown physical fields in isogeometric analysis provides solution for the integration of computer aided design and engineering, and also promotes the development of approximation theory with splines. Quasi-conforming (QC) technique is initially developed within traditional finite element framework by Prof. L.M. Tang. The major advantage of QC technique in the formulation is that the approximate space for displacements and strains are separately defined and the displacement-strain equation is transformed from partial differential form into weakened integration form. Inspired by isogeometric method, the quasi-conforming techniques are developed into exact geometry based quasi-conforming analysis method (EGQC) which uses NURBS based geometry as input model rather than traditional mesh. The contributions of the proposed EGQC method are listed as below. First, the displacements and strains are separately approximated according to the property of solved problem to achieve better performance. Second, the basis functions to describe the unknown physical fields are chosen according to the solved problems which are not limited to splines. Applications with the EGQC method on structural analysis have been developed. First the algorithms for analysis of beam structure with Euler and Timoshenko beam theories are proposed. The polynomial basis is used in simulation of Euler beam to improve the computational efficiency [1]. An order-reduction method with Timoshenko beam theory is proposed to cure the locking problem [2]. The method behaves great in simulation of beam structure and is expanded to the simulation of Reissner-Mindlin shell problems. In future works the EGQC method will be expanded to problems with extra constrains for the solution space, such as the simulation for incompressible material. References [1]Ping Hu Yang Xia Changsheng Wang, Exact geometry based quasi-conforming analysis for Euler-Bernoulli beam. Theoretical & Applied Mechanics Letters, 2012, 2(5), 6-9. [2]Ping Hu, Qingyuan Hu, Yang Xia, Order reduction method for locking free isogeometric analysis of Timoshenko beams, Computer Methods in Applied Mechanics and Engineering, Volume 308, 2016, Pages 1-22.

Numerical Simulations of the Ignition Dynamics in an Annular Combustor

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ABSTRACT

An annular combustor which comprises multiple swirling injectors is an universal and crucial configuration for modern aero-engines. In present work, the transient flame front propagation during ignition process in a laboratory-scale annular combustor is numerically investigated in Large-eddy simulation (LES) and RANS to understand the ignition dynamics. The annular combustor comprises sixteen swirling injectors injecting lean premixed propane/air mixtures and two transparent quartz concentric cylindrical walls of the combustion chamber, which provides optical access to high-speed imaging to diagnosis the chemiluminescence of flame front. Various experiments have been conducted on the annular combustor which provide the database to validate the numerical results. Three stages of ignition process are distinctly exposed towards understanding of gas turbine ignition. The ignition process is numerically investigated by LES and RANS with detailed chemistry in this paper. The factors, such as fuel to air ratio and flow characteristics, influencing light-round ignition process are extensively explored. The numerical results of LES and RANS are well consistent to each other. Meanwhile, the ignition sequences of light-round process are compared with experimental data, which show an overall good agreement. The non-symmetric circumferential flame propagation is observed in simulations and experiments, which is induced by circumferential flow characteristics due to the arrangement of multiple swirling injectors. The circumferential flow characteristics and flame/flow interactions are analyzed in the numerical simulations. The simulations reveal that the turbulent wrinkling and thermal expansion are the main effects to the flame front propagation. The wrinkling factor of the flame front is calculated to qualify the influence of flame/turbulence interaction in the flame front propagation, which is hardly obtained by experiments. The thermal expansion rate across the flame front is studied by the temperature distribution. The simulations enable detailed data analysis compared to experimental measurements. The light-around time and circumferential flame propagation speed are quantitatively calculated to characterize the ignition dynamics during the light-around ignition.

2D Analysis of Cracked Viscoelastic Media Using Singular Element

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ABSTRACT

In this paper, crack problem in linear viscoelastic material is studied numerically by using a singular element which was derived based on the Symplectic Eigen Solution (SES) for crack. Firstly, the fundamental equations of 2D viscoelastic problem are transformed into a series of elastic crack problems by using the method of precise time-domain expanding algorithm. These time independent elastic crack problems are connected through the time-domain expanding coefficients of displacement and stress in a recursive manner. Secondly, the elastic crack problems are solved by using finite element method and the singular element is applied to solve the stress singularity problem. The circle singular element occupies the area around the crack tip and is connected to the conventional elements meshed in the other area through export nodes. Mesh refinement near the crack tip is unnecessary and hence the computational costs are significantly reduced. Taking advantages of the proposed method, the viscoelastic fracture parameters such as stress intensity factor, crack opening and sliding displacement and strain energy release rate are all related to the symplectic eigen expanding coefficients and can be solved directly without any post-processing. Finally, numerical examples are provided to demonstrate the proposed method. Numerical predictions are also compared with those obtained by other numerical methods, such as, extended finite element method, enriched finite element method, boundary element method and numerical manifold method. The comparisons show that the present method is convenient, accurate and efficient.

A Stress State Dependent Constitutive Model for Finite Deformation of Soft Elastomers

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ABSTRACT

Predicting the constitutive behavior of finite deformation of soft elastomers under complex stress state is a long-standing challenge because a large number of constitutive models calibrated from uniaxial stress state cannot accurately characterize the responses under complex stress state. Therefore, we developed a stress state dependent constitutive model based on a new microscopic picture, in which the stress is decomposed into two parts: one comes from cross-linked network and another comes from entangled network. Then the experimental results of vulcanized rubber, natural rubber, Entec Enflex S4035A thermoplastic elastomer (TPE), silicone rubber and Tera-PEG gel under the uniaxial, biaxial and pure shear loading conditions are used to calibrate and verify the proposed constitutive model. Meanwhile, a comparison is made with other similar constitutive models (extended tube model and nonaffine network model). It is shown that the proposed model can not only capture softening with a stress plateau, hardening with a sharp rise in stress, but also can accurately characterize the constitutive behaviors of soft rubberlike material under complex stress state with only three material parameters. Furthermore, the stress state dependent constitutive model can accurately simulate the deformation process of the complex structure, thus proving that the proposed model have great potential applications in the area of soft robots, soft electronics and polymer manufacture.

Geometrically Nonlinear Finite Element Method Based on the Willis-Form Equations

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ABSTRACT

It has been proved that linear elastic equations for inhomogeneous media are in Willis-forms with a displacement coupling term related with the gradient of pre-stresses [1]. This has also been verified by an experiment on rotational springs [2]. Since the pre-stress is crucial to finite deformation analysis, we propose a new geometrically nonlinear finite element method in updated Lagrangian formulation based on the Willis-form equations. This method is featured with an additional stiffness matrix, which contains the gradient of pre-stress of previous load step. In this way, efficient Newton-Raphson iteration is conducted by using a secant stiffness matrix. Acknowledgement This work is supported by National Science Foundation of China with grant number 11672144. References [1] ZH Xiang and RW Yao. Realizing the Willis equations with pre-stresses. *Journal of the Mechanics and Physics of Solids*, 87, 2016: 1-6. [2] RW Yao, HX Gao, YX Sun, XD Yuan, ZH Xiang. An experimental verification of the one-dimensional static Willis-form equations. *International Journal of Solids and Structures*, 2017, doi.org/10.1016/j.ijsolstr.2017.06.005.

A 3D Mesoscopic Model for the Dynamic Behavior of an Al/PTFE Composite

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ABSTRACT

Abstract: reactive materials or impact-initiated materials are known to be reactive under dynamic impacting and released large quantity of energy. As a typical impact-initiated composite, Al/PTFE composite has been investigated extensively those years. The mechanical behavior of an Al/PTFE composite under dynamic loading with numerical simulation and experiments. The composite was produced with powder mixed, suppression and sintering. The microstructure of the composite was obtained with micro CT facility, a 3D mesoscopic model was established by following a series of image processing procedures. Gas gun launched impact experiments were conducted to investigate the mechanical behavior of composite under dynamic loading. The results of simulations agreed well with the experiment results. It is indicated that the 3D mesoscopic model procedure used in this paper is an efficient method to predict the dynamic behavior of composites under impact loading.

Large-Eddy Simulation of a Screeching Axisymmetric Jet in the Helical Mode

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ABSTRACT

Large eddy simulation is performed for investigating the screech noise generation and shock-vortex interactions of a screeching axisymmetric jet in the helical C mode issuing from a convergent nozzle at a nozzle pressure ratio of 3.4. The nozzle pressure ratio, exit diameter and lip thickness of nozzle are the same as the experiment condition in [1]. The Favre filtered compressible Navier–Stokes equations in cylindrical coordinates have been solved by using a finite difference method. The large eddy simulation code employs a seven-order weighted essentially non-oscillatory scheme [2] for the convective fluxes, a sixth-order centered difference approach for the viscous fluxes, and a four-stage third-order strong-stability-preserving Runge–Kutta technique in time. The simulated mean velocity field, shock cell structures and screeching frequency are all in good agreement with the experimental measurements. The large helical vortex structures appear in the jet shear layer which coincide with the helical screeching mode. It is also found in numerical results that shock structures oscillate periodically with the screeching frequency. The helical shock motions of the forth shock structure is complicated. In our research, the organized vortices in the jet shear layer change shock formations by modifying the sonic line. The fluctuating velocities of numerical data have been analysed by proper orthogonal decomposition(POD). The first two modes of POD containing more energy than other modes. The mode 1 and mode 2 would look visually the same but a spatial phase shift ensures orthogonality between mode 1 and 2. The POD results in several different planes indicate that the helical vortices in jet shear layer are the dominant dynamic flow structures and they are related with screeching sound waves strongly. [1] Edgington-Mitchell, D., et al. (2014). "Coherent structure and sound production in the helical mode of a screeching axisymmetric jet." *Journal of Fluid Mechanics* 748: 822-847. [2] Balsara, D. S. and C.-W. Shu (2000). "Monotonicity Preserving Weighted Essentially Non-oscillatory Schemes with Increasingly High Order of Accuracy." *Journal of Computational Physics* 160(2): 405-452.

Development of a Transferable Reactive Force Field of P/H Systems: Application to the Chemical and Mechanical Properties of Phosphorene

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ABSTRACT

We developed ReaxFF parameters for phosphorus and hydrogen to give a good description of the chemical and mechanical properties of pristine and defected black phosphorene. ReaxFF for P/H is transferable to a wide range of phosphorus and hydrogen containing systems including bulk black phosphorus, blue phosphorene, edge-hydrogenated phosphorene, phosphorus clusters and phosphorus hydride molecules. The potential parameters were obtained by conducting global optimization with respect to a set of reference data generated by extensive ab initio calculations. We extended ReaxFF by adding a 60° correction term which significantly improved the description of phosphorus clusters. Emphasis was placed on the mechanical response of black phosphorene with different types of defects. Compared to the nonreactive SW potential,¹ ReaxFF for P/H systems provides a significant improvement in describing the mechanical properties of the pristine and defected black phosphorene, as well as the thermal stability of phosphorene nanotubes. A counterintuitive phenomenon is observed that single vacancies weaken the black phosphorene more than double vacancies with higher formation energy. Our results also showed that the mechanical response of black phosphorene is more sensitive to defects in the zigzag direction than that in the armchair direction. In addition, we developed a preliminary set of ReaxFF parameters for P/H/O/C to demonstrate that the ReaxFF parameters developed in this work could be generalized to oxidized phosphorene and P-containing 2D van der Waals heterostructures. That is, the proposed ReaxFF parameters for P/H systems establish a solid foundation for modelling of a wide range of P-containing materials.

A 2D Local Discontinuous Galerkin Finite Element Method Solution of the Richards's Equation

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ABSTRACT

Unsaturated flows in porous media influenced by hydraulic conductivity and capillary pressure are governed by the Richards's equation. Many available numerical Richards's equation solvers are based on conforming finite element methods, which could experience numerical difficulties when soil water content undergoes abrupt changes and/or in the presence of natural heterogeneities in porous media. In light of such challenges, a two-dimensional numerical solver is formulated based on the local discontinuous Galerkin finite element method (LDG-FEM) -- a class of finite element method that employs piecewise continuous trial spaces and allows solution discontinuity across element boundaries. Soil water content measurement will be acquired from the National Oceanic and Atmospheric Administration (NOAA) for model validation. Extension of this LDG solver as a general framework in solving other convection-diffusion problems is expected in future.

Electromechanical Response and Effective Properties of Piezoelectric Fiber Composite with Arbitrary Shape Inclusion

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ABSTRACT

The piezoelectric fiber composite has achieved great application in vibration control of aeronautic and aerospace structures, which contains an active layer constructed by piezoceramic fibers embedded in polymer matrix. In this paper, an analytical framework based on the complex potential theory and the generalized self-consistent method has been developed to predict the electromechanical fields and the effective properties of piezoelectric fiber composite. A three-phase model is presented, which assumes a representative cell containing an arbitrary shape piezoelectric fiber and non- piezoelectric matrix is embedded in infinite equivalent piezoelectric composite. Both of in-plane strain with transverse electric fields and anti-plane shear with in-plane electric fields are considered. Firstly, a new conformal mapping method is proposed to translate arbitrary two connected domain into annular domain, and arbitrary simply connected domain into circle domain. Then, the general solutions of the complex potential for each component can be expressed in series form with unknown coefficients. The continuity conditions of the interfaces and the homogeneous conditions are used to build up a set of equations to determine the unknown coefficients. After the complex potentials are solved, the exact electromechanical response and effective properties of piezoelectric fiber composite with arbitrary shape inclusion are obtained. It is shown that the inclusion shape has a significant influence on the stress and electric field distribution at the interface between the matrix and piezoelectric fibers. Furthermore, the proposed analytical framework provides a powerful instrument for solving the related problems about fibrous composites with imperfect interfaces or with coated phase.

Interfacial Stress Evolution during the Isothermal Growth of Mixed Oxide Layer in Thermal Barrier Coating System

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ABSTRACT

Abstract: Thermal barrier coating system (TBCs) is widely used in hot-section component parts of gas turbine. A prepared TBCs typically consists of a bond coat (BC) and a ceramic top coat (TC). An additional thermal growth oxidation (TGO) layer will form in pre-treatment or in service. During TGO growth, a layer of α -Al₂O₃ appears first, which provides oxidation protection. Then with time evolution, mixed oxide (MO) forms. MO grows much faster than α -Al₂O₃. It expands significantly and is one of main causes for the failure of TBCs. During the isothermal growth of MO in TBCs, severe stresses are generated and may induce micro-cracks and delamination. This work analyzes the local stress evolution around the convex morphology of MO by establishing the evolution equations on stress. A modified finite difference method is implemented to solve the problem. The effects of growth rate and volume expansion ratio of MO on the local stresses are considered. Through numerical analysis, we found that the stress induced by the growth of MO is much larger than that of α -Al₂O₃. The radial stress of α -Al₂O₃/MO interface gradually changes from compression to tension with the growth of MO. The radial tensile stress results in the initiation of the delamination. The growth of MO also induces the hoop tensile stress near the TC/MO interface and leads to the occurrence of the micro-cracks, which is in accordance with the experimental observation. Key words: local stress evolution, thermal barrier coating system, mixed oxide, oxidation growth, sphere model

In Situ Observation and Numerical Simulation of the Thermal Distortion during Direct Energy Deposition Process

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ABSTRACT

Part distortion is a technical bottleneck in the field of metal additive manufacturing, which depends on the thermo-mechanical behavior the material experienced during deposition process. This study successfully obtained the continuous full-field strain of a Ti-6Al-4V thin-wall during the direct energy deposition additive manufacturing process using digital image correlation (DIC) method. The finite element method was established based on the same deposition process with the experiments. The numerical simulation results agree well with experiments. The longitudinal strain increased rapidly to tensile strain as the laser beam approached, whereas the vertical strain decreased rapidly to a compressive strain and gradually transformed to tensile strain. The strains accumulated and rose periodically for the first several layers, which then decreased periodically during the following deposition. The strain accumulation behavior varied with the location of the deposited part, which caused the uneven distortion both in longitudinal and vertical directions. Increasing interlayer cooling time could significantly reduce the transient distortion of the deposited part during deposition, while it was not good for the final distortion. The in-situ strain field of additive manufactured part obtained in this study can be an effective validation for theoretic and computation studies, which also provides valuable guidance for real-time monitoring and controlling of stress and distortion for industry production.

Topology Optimization Analysis of Tensegrity Torus Based on Niche Genetic Algorithm

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ABSTRACT

An absolute self-balancing cable dome can be created by adopting tensegrity torus as ring girders. A topology optimization method based on improved genetic algorithm with the sharing function niche mechanism, pre-selection niche mechanism and adaptive technique is proposed by considering the flexibility and mechanical properties of tensegrity torus. The minimum structural weight is taken as the optimal objective of the method. The four constraint conditions of the method are feasible integral structural pre-stressing, none cross collision of bars, constraint of members stress and limitation of structure displacements. In order to obtain the static analysis results of tensegrity torus of different topological conditions efficiently, a self-compiled program of vector form intrinsic finite element is applied in the algorithm. Finally, the analysis results of several examples of different spans and topological conditions solved by ANSYS prove the effectiveness of the proposed computing method. The improved niche genetic algorithm provides a new computing method for the topology optimization of tensegrity torus?

A New MMC-based Isogeometric Topology Optimization Using R-functions and Collocation Schemes

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ABSTRACT

A new isogeometric topology optimization (TO) method based on moving morphable components (MMC) is presented, where R-functions are used to represent the topology description functions (TDF) to overcome the C1 discontinuity problem of the overlapping regions of components. Three new ersatz material models based on uniform, Gauss and Greville abscissae collocation schemes are used to represent both the Young's modulus of material and the density field based on the Heaviside values of collocation points. Three benchmark examples are tested to evaluate the proposed method, where the collocation schemes are compared as well as the difference between isogeometric analysis (IGA) and finite element method (FEM). The results show that the convergence rate using R-functions have been improved in a range of 17%-40% for different cases in both FEM and IGA frameworks, and the Greville collocation scheme outperforms the other two schemes in the MMC-based TO.

COMPUTATIONAL HOMOGENIZATION SIMULATION ON STEEL REINFORCED RESIN USED IN THE INJECTED BOLTED CONNECTIONS

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Key words: Steel reinforced resin, linear Drucker-Prager plastic model , Finite element simulation, Computational homogenization.

Abstract: Injected bolts are regarded as a suitable alternative for a renovation of riveted connections of large span structures. Recently, the injected material, epoxy resin is modified at TU Delft by adding the steel shots to improve injected bolts performance suitable for reusable composite (steel-concrete) structures. The shots serves as reinforcement into epoxy resin serving as matrix. Increase of compressive strength and stiffness, and improvement of creep characteristics of the reinforced injected materials are expected. In a bolt hole the reinforce resin appears in confinement environment and will improve performance of connections exposed to monotonic and cyclic loading. In this paper, numerical homogenization, where combined non-linear isotropic/kinematic cyclic hardening model is employed to define the steel plasticity, linear Drucker-Prager plastic criterion was used to simulate resin damage, and the cohesive surfaces reflecting the relationship between traction and displacement at the interface were employed to simulate the steel-resin interface, is conducted to predict the tensile and shear behaviour of steel reinforced resin after validated by compressive material test results. The friction angle β , the ratio of the yield stress in triaxial tension to the yield stress in triaxial compression K , and the dilation angle ψ of linear Drucker-Prager plastic model are obtained based on experiments and numerical homogenization simulation. The confinement effects on steel reinforced resin could be effectively simulated. Finite element simulations on unconfined/confined steel reinforced resin material tests were conducted to validate the material parameters proposed in this paper. A good agreement is observed, indicating the model and parameters proposed in this paper could be effectively used in the finite element simulation of injected bolts.

1 INTRODUCTION

Injected bolts are regarded as a suitable alternative for a renovation of fitted bolts, riveted or preloaded connections of large span structures [1–3]. A hole is included in the head of the bolt in order to inject the bolt-hole clearance with a resin. After injection and curing of the resin, the connection is slip resistant. Recently, the injected material, epoxy resin is modified at TU Delft by adding the steel shots (reused after abrasive blast cleaning of steel surface) to increase initial stiffness of the connection for reusable composite (steel-concrete) structures[4]. The shots serves as reinforcement of an epoxy resin serving as matrix. Additional increase of compressive strength and expected improvement of creep characteristics of the reinforced injected material, especially in an oversized bolt clearance connection, will improve performance of connections exposed to monotonic and cyclic loading.

Besides the experimental research, numerical simulations may play an important role in the qualification and certification of short- and long- term behaviour of injection bolts. The material models of resin/steel reinforced resin are investigated before conducting finite element simulation on structural elements containing connection with injection bolts. However, the material behaviour of reinforced resin depends on the type of resin, type of the reinforcing material, the volume fraction of resin and steel shots and the size of the hole clearance. It is appropriate to adopt a multi-scale analysis to determine the mechanical properties of the steel-reinforced resin. Numerical homogenization method [5], which could accurately consider the geometry and spatial distribution of the phases, and also could precisely estimate the propagation of damage in order to accurately predict the failure strength, is considered to be an effective modelling tool for analysis of steel reinforced resin performance. Fish et al. [6–9] successfully use the statistically computational homogenization methods to predict the macroscopic behaviour of concrete, FRP material and even femur fracture. Xin et al. [10–12] adopted a multi-scale analysis in determining mechanical properties of pultruded GFRP laminates and successfully predict the mechanical behaviour of a pultruded GFRP bridge deck. Gonzalez and LLorca [13] analysed the mechanical response of a unidirectional FRP subjected to transverse compression. Vaughan and McCarthy [14] investigate the effect of fiber–matrix debonding and thermal residual stress on the transverse damage behavior of unidirectional FRP.

Computational homogenization methods of fine scale models provide a pathway to use high fidelity models to predict macroscopic mechanical responses of steel reinforced resin. However, the high fidelity numerical homogenization methods are reported computationally expensive [15–18]. The hierarchical strategy, where experimental results and high fidelity model (HFM) are employed to train a low fidelity model (LFM) and to supplement experimental database is adopted to model the material behaviour of steel reinforced resin [18]. The performance of the steel reinforced resin is effectively predicted by an elaborate but computationally inexpensive low fidelity model identified by a more fundamental but computationally taxing high fidelity model, which has been calibrated to the experimental results.

In this paper, first-order numerical homogenization is employed as high fidelity model, where combined non-linear isotropic/kinematic cyclic hardening model is employed to define the steel plasticity, linear Drucker-Prager plastic criterion was used to simulate resin damage, and the cohesive surfaces reflecting the relationship between traction and displacement at the interface. The linear Drucker-Prager plastic model is used as low fidelity model. The friction angle β , the ratio of the yield stress in triaxial tension to the yield stress in triaxial compression K , and the dilation angle ψ of linear Drucker-Prager plastic model are obtained based on experiments and

numerical homogenization simulation. Finite element simulations on unconfined/confined steel reinforced resin material tests were conducted to validate the proposed material parameters. This research may contribute to numerical simulation and practical design of injection bolts.

2 COMPUTATIONAL HOMOGENIZATION

2.1 Computational Homogenization and Periodic Boundary Condition

The link between micro-scale and macro-scale behaviour could be established based on Hill-Mandel computational homogenization method. The macro-scale Cauchy stress is obtained by averaging the micro scale Cauchy stress, in the unit cell domain, expressed as below [5]:

$$\sigma_{ij} = \frac{1}{|\Theta|} \int_{\Theta} \tilde{\sigma}_{ij} d\Theta \quad (1)$$

where: σ_{ij} is the macro-scale Cauchy stress, $\tilde{\sigma}_{ij}$ is the micro-scale Cauchy stress, Θ is the domain of the unit cell.

The boundary was implemented by so called “mixed boundary conditions” via constraint equations, is expressed by the following equations [5,19]:

$$\int_{\partial\Theta_Y} (u_i^f(x, y) - \varepsilon_{ik}^c y_k) N_j^\Theta d\gamma_Y = 0 \quad (2)$$

$$|u_i^f(x, y) - \varepsilon_{ik}^c y_k| N_j^\Theta \leq Tol \quad (3)$$

where: N_j^Θ is the unit normal to the unit cell boundary $\partial\Theta_y$.

2.2 Material Constitutive law

(1) Steel

The combined non-linear isotropic/kinematic cyclic hardening model is employed to define the steel plasticity [20]. The yield surface generally consists of two components, (i) a nonlinear kinematic hardening component, which describe the translation of the yield surface in stress space through the back-stress; and (ii) an isotropic hardening component, which describe the change of the equivalent stress defining the size of the yield surface as a function of plastic deformation. The pressure-independent yield surface is defined as below:

$$F_1 = f(\sigma - \alpha) - \sigma^0 = 0 \quad (4)$$

where σ^0 is the yield stress and $f(\sigma - \alpha)$ is the equivalent Mises stress with respect to the back-stress α . The non-linear kinematic/isotropic hardening is employed to describe the translation of the yield surface in stress space. The kinematic hardening is specified by half-cycle input material data. For each input material data point $(\sigma_i, \varepsilon_i^{pl})$, a value of back-stress α_i is obtained from the input data as:

$$\alpha_i = \sigma_i - \sigma_i^0 \quad (5)$$

where σ_i^0 is the user-defined size of the yield surface at the corresponding plastic strain for the isotropic hardening component. Integration of the backstress evolution laws over a half cycle yields the expression:

$$\alpha = \sum_{k=1}^N \left[\frac{C_k}{\gamma_k} \left(1 - e^{-\gamma_k \varepsilon_i^{pl}} \right) \right] \quad (6)$$

where N is number of back-stress, C_k and γ_k are material parameters and calibrated through material data.

(2) Resin

The plastic behaviour of resin was assumed to be governed by the linear Drucker-Prager model. The yield surface of the linear Drucker-Prager model [20] is given below.

$$F_2 = t - p \tan \beta - d = 0 \quad (7)$$

$$t = \frac{1}{2} q \left[1 + \frac{1}{K} - \left(1 - \frac{1}{K} \right) \left(\frac{r}{q} \right)^3 \right] \quad (8)$$

where β is the slope of the linear yield surface and is commonly referred as the friction angle of the material, d is the cohesion of the material, K is the ratio of the yield stress in triaxial tension to the yield stress in triaxial compression, and controls the dependence of the yield surface on the value of the intermediate principal stress. The flow potential of linear Drucker-Prager model is chosen as below equations:

$$G = t - p \tan \psi \quad (9)$$

where ψ is the dilation angle.

(3) Steel-Resin Interface

The cohesive surfaces reflecting the relationship between traction and displacement at the interface were used to simulate the steel-resin interface. The cohesive element is always subjected to complicated loading condition; the quadratic stress failure criterion [20] is used to evaluate the initial damage.

$$\left\{ \frac{\langle t_n \rangle}{t_n^0} \right\}^2 + \left\{ \frac{t_s}{t_s^0} \right\}^2 + \left\{ \frac{t_t}{t_t^0} \right\}^2 = 1 \quad (10)$$

where: t_n , t_s and t_t are traction components related to pure modes *I*, *II* and *III*, t_n^0 , t_s^0 and t_t^0 are interfacial strength of pure modes *I*, *II* and *III*. In the damage evolution period, the interfacial stiffness degraded from initial K_0 to $(1-d)K_0$, where d is a damaged variable. The Benzeggagh-Kenane fracture criterion (BK Law) [20,21] is particularly used to predict damage propagation of mixed-mode loadings in terms of the critical fracture energies during deformation purely along the first and the second shear directions are the same.

$$G^C = G_n^C + (G_s^C - G_n^C) \left\{ \frac{G_s + G_t}{G_n + G_s + G_t} \right\}^\eta \quad (11)$$

where: G_n , G_s , and G_t are the corresponding energy release rates under pure modes *I*, *II*, and *III*, the additional subscript “*C*” denotes critical case, which can be determined based on a standard fracture toughness test and η is a material parameter.

3. STRESS-STRAIN RELATIONSHIP OF RESIN

The uniaxial compressive behaviour of resin is described by combining the damage mechanics and Ramberg-Osgood relationship [22], as below:

$$\sigma = (1-D)\sigma^{R-O}(\varepsilon) \quad (12)$$

$$\varepsilon = \frac{\sigma^{R-O}}{E} + K \left(\frac{\sigma^{R-O}}{E} \right)^n \quad (13)$$

where: D is damage variable. The damage variable is defined as below:

$$D = \begin{cases} 0 & \varepsilon < \varepsilon_0^f \\ \frac{\varepsilon - \varepsilon_0^f}{\varepsilon_u^f - \varepsilon_0^f} & \varepsilon \geq \varepsilon_0^f \end{cases} \quad (14)$$

where: ε_0^f is plastic strain at fracture initiation, ε_u^f is the plastic strain at the failure. The fracture initiation strain ε_0^f is assumed to be the corresponding strain at the peak load while the failure strain is obtained by extended the softening stage. The parameters relationship is fitted based on the experimental results before damage occurred. The fitted material parameters are listed in Tables 1.

Table 1 Ramberg-Osgood Relationship Parameters of Resin and Steel-reinforced Resin

Item		K	n	R ²	ε_0^f (%)	ε_u^f (%)
Resin	Nominal Stress	6.07×10^{11}	8.27	0.98	1.01	4.07
	True Stress	1.62×10^{16}	10.62	0.95	1.03	1.03

The friction angle β , the ratio of the yield stress in triaxial tension to the yield stress in triaxial compression K, and the dilation angle ψ is calculated based on experiments and listed in Table 2.

Table 2 Material Parameters of linear Drucker-Prager model

Material	Associated flow			Non-dilatant flow		
	β	K	ψ	β	K	ψ
Resin	12.16^0	0.92	12.16^0	12.18^0	1.00	0^0
Steel reinforced resin	49.80^0	0.78	49.80^0	52.04^0	1.00	0^0

4. COMPUTATIONAL HOMOGENIZATION

It is very difficult to make a dog-bone shape tensile specimens in order to experimentally obtain tensile behaviour. The computational homogenization method provide an alternative way to obtain the tensile and shear behaviour numerically after validating the multiscale model with compressive test results. The unit cell is shown in Fig. 1. Material model and parameter used in Section 3 is employed to simulate the resin behaviour in the computational homogenization modelling. S235 grade steel is employed to describe the behaviour of steel shot based on Eurocode EN 1993-1-1 nominal data, [23]. The ‘‘mixed periodic boundary conditions’’ are applied to the unit cell via constraint equations. Surface cohesive model is used to describe the interface behaviour between steel and resin. The interface parameters are calibrated based on compressive test results. The normal interface stiffness is calibrated as 5.53×10^5 N/mm³, and the

shear interface stiffness is calibrated as $2.01 \times 10^5 \text{ N/mm}^3$. The normal interface strength obtained after the calibration is 40.8 MPa. The shear interface strength is calibrated to 41.5 MPa. The normal critical fracture energies G_n^c is determined as 0.04 kJ.mm^{-1} , and the shear critical fracture energies G_s^c and G_t^c is determined as 0.45 kJ.mm^{-1} . The material parameter is assumed to be 1.8 based on references [11,12]. The viscosity coefficient for the cohesive surface is assumed to be 0.001 s.

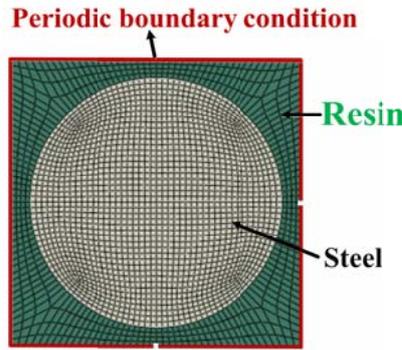


Figure (1): Unit cell of steel reinforced resin

Compressive stress-strain relationship comparisons between numerical homogenization and experiments of unconfined steel reinforced resin is shown in Fig.2. The macro scale stress is obtained based on Eq.(1), so the homogenization results is compared with true stress and strain relationship. A good agreement is observed, indicating it is reliable to use computational homogenization method to predict the tensile and shear behaviour of steel reinforced resin.

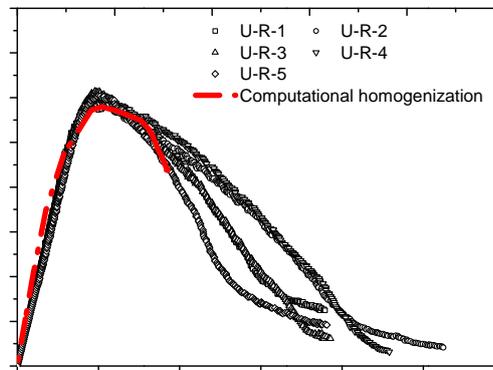
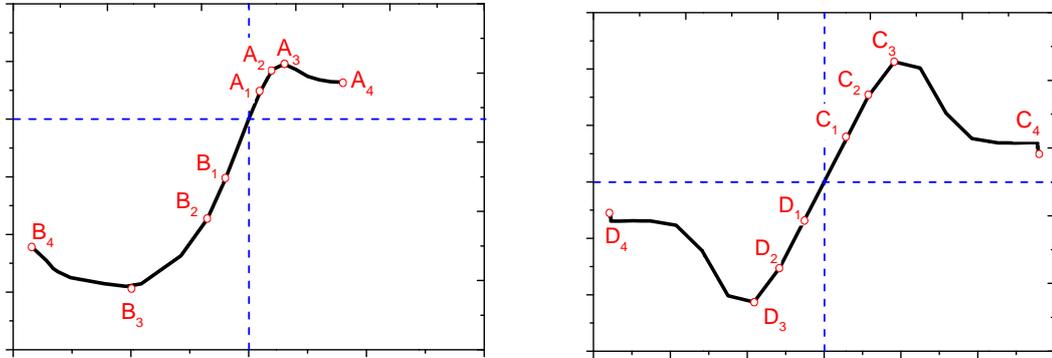


Figure (2): Stress-strain relationship comparisons between numerical homogenization and experiments of unconfined steel reinforced resin

The uniaxial stress and strain relationship, shear stress and strain relationship based on numerical homogenization method is shown in Fig. 3. The ultimate tensile strength of steel reinforced resin is 39.8Mpa. The Mises stress distribution and deformation of unit cell is shown in Fig. 4 and Fig .5 at different stages in Fig. 3. The principal plastic strain at the failure of the unit cell is shown in Fig. 6. The numerical multiscale simulation indicated that the damage and failure of steel reinforced resin is governed by the resin and interface while the steel is in the elastic stage during uniaxial and shear loading. The friction angle β , the ratio of the yield stress in triaxial

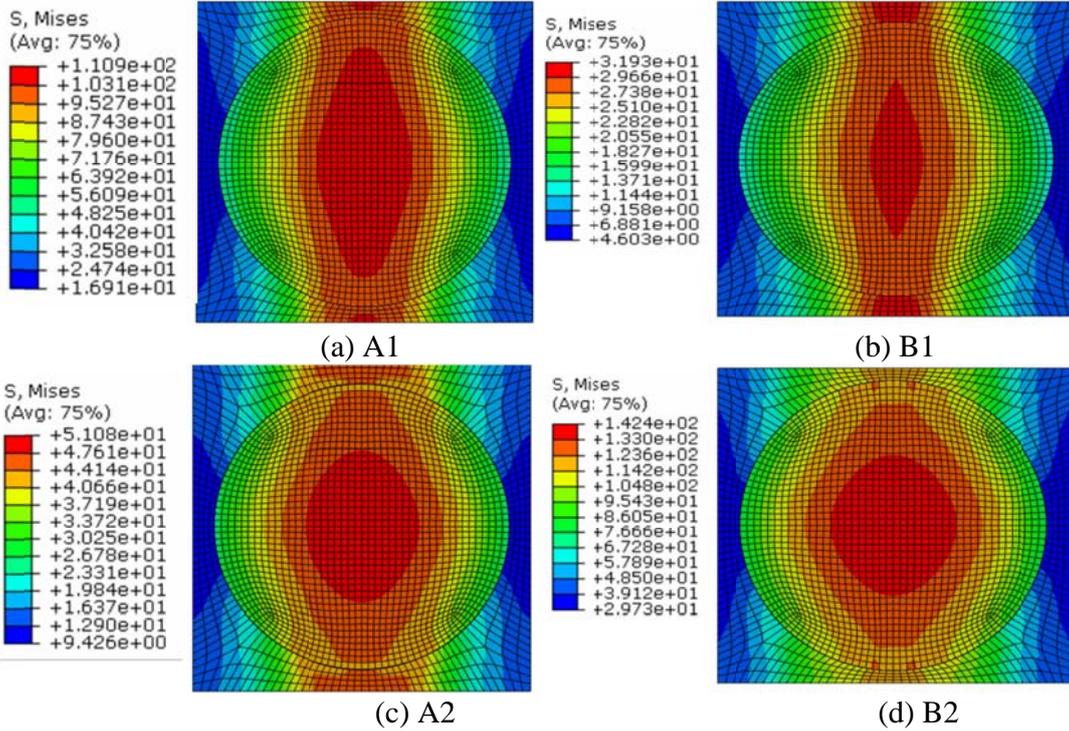
tension to the yield stress in triaxial compression K , and the dilation angle ψ is calculated based on multiscale simulation results. The steel reinforced resin material parameters of the linear Drucker-Prager model is summarized in Table 2.



(a)

(b)

Figure (3): Stress-strain relationship of steel reinforced resin calibrated by the numerical homogenization



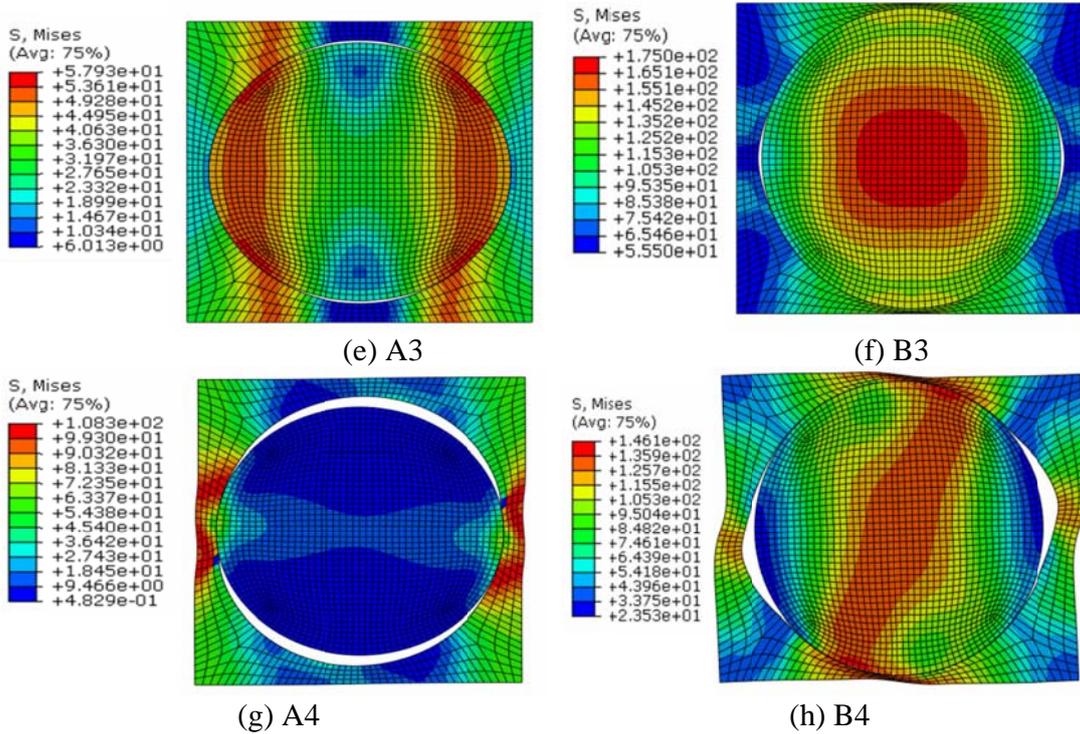
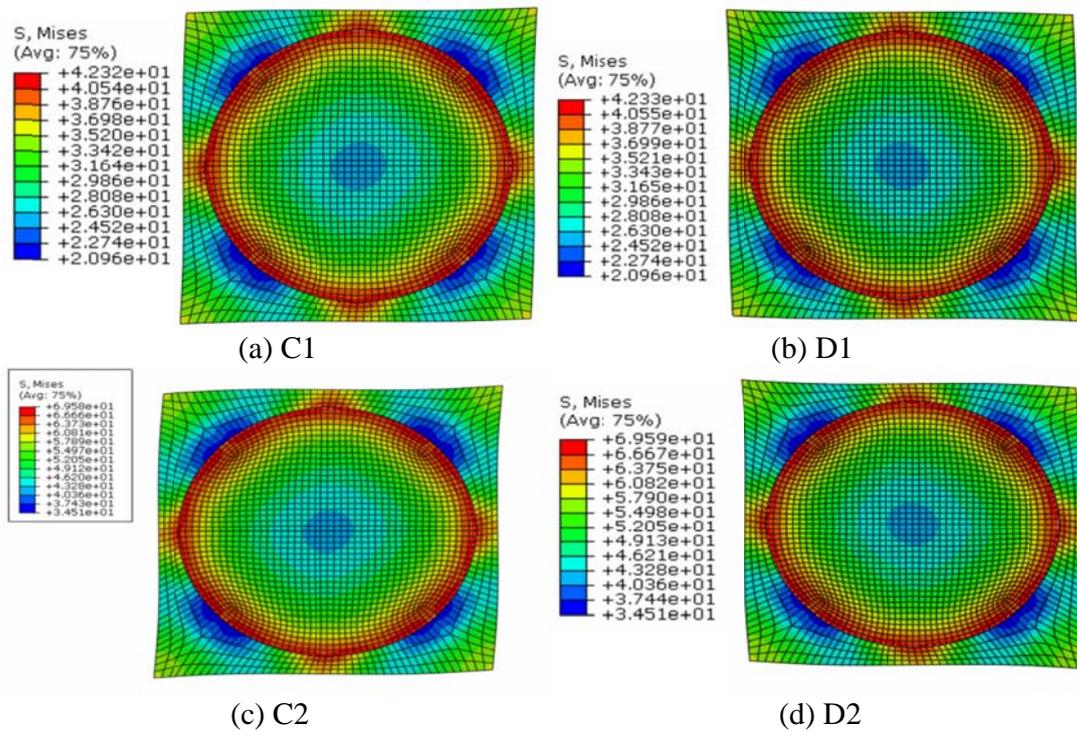


Figure (4): Mises stress distribution of unit cell under uniaxial loading in compression A1 to A4 and in tension B1 to B4 (in Fig.2)



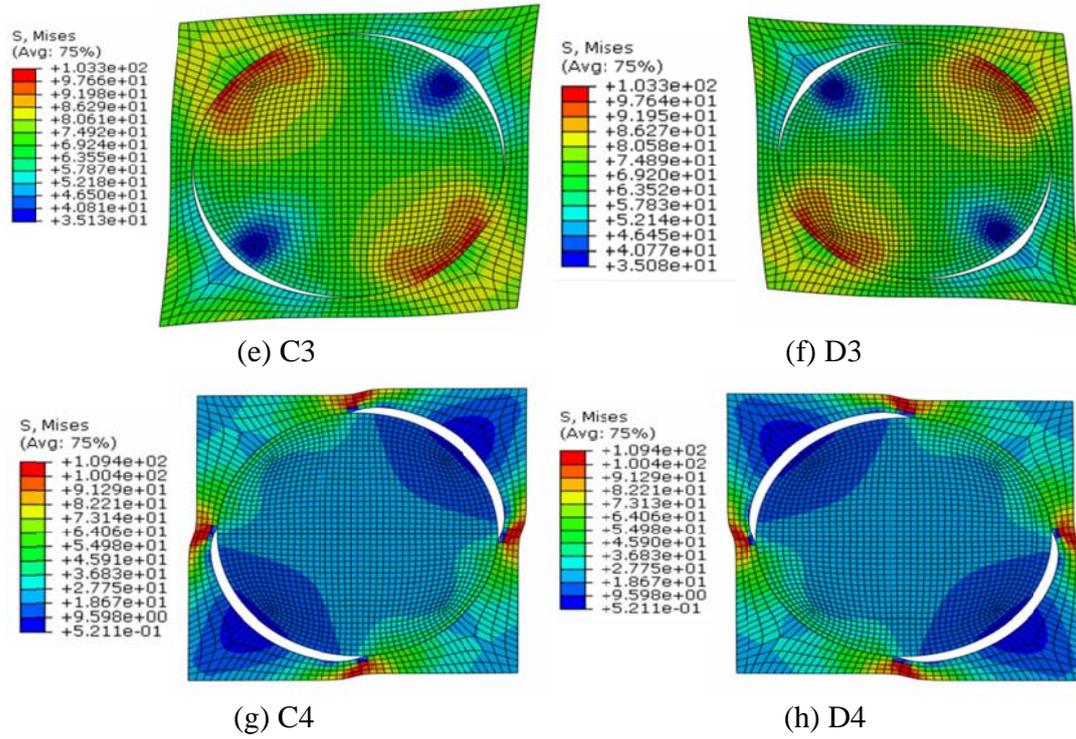


Figure (5): Mises stress distribution of unit cell under shear loading under shear loading C1 to C4 and D1 to D4 (in Fig.2)

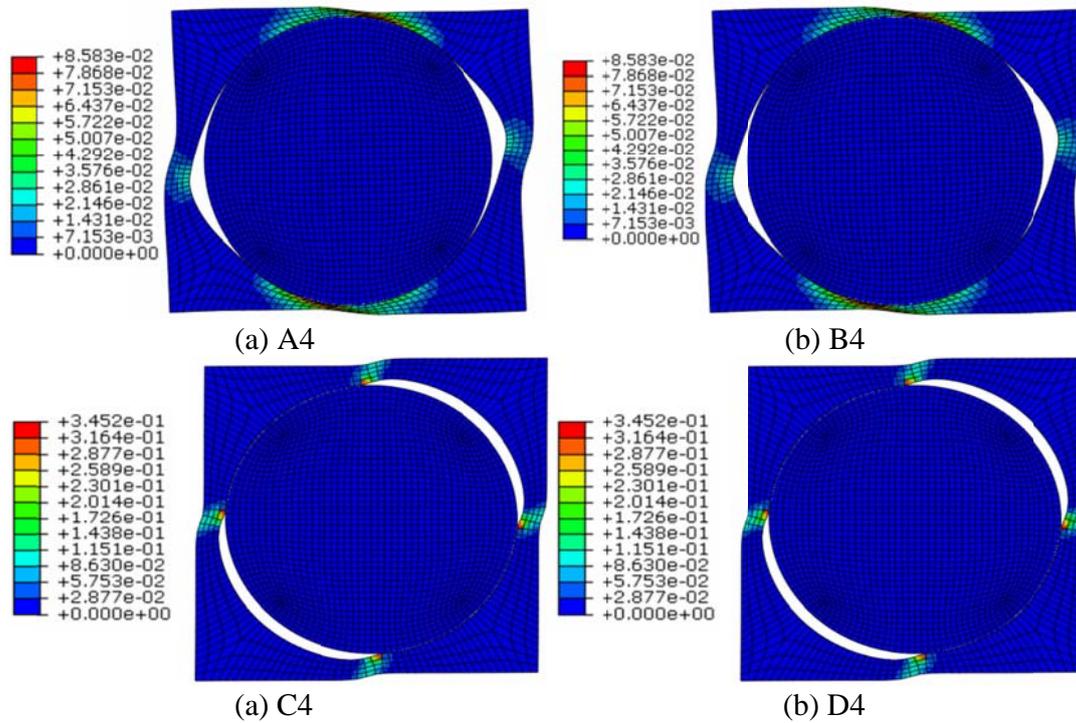
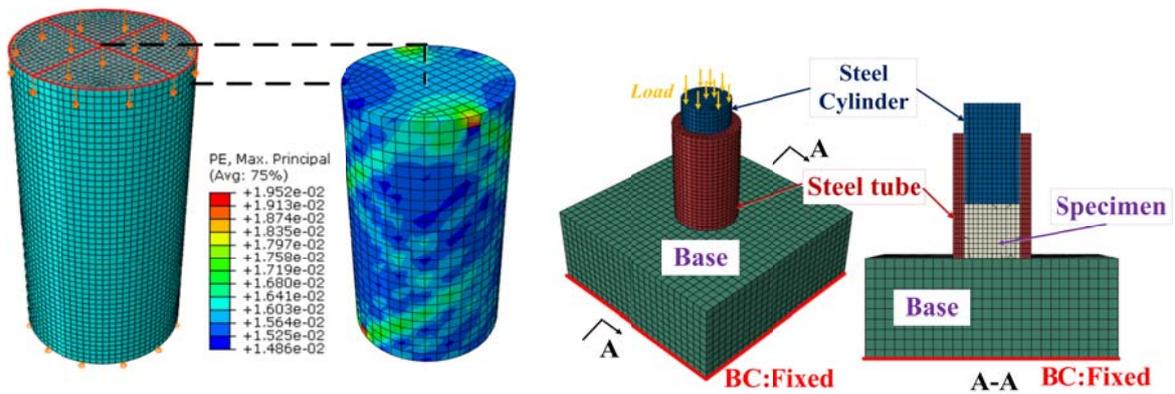


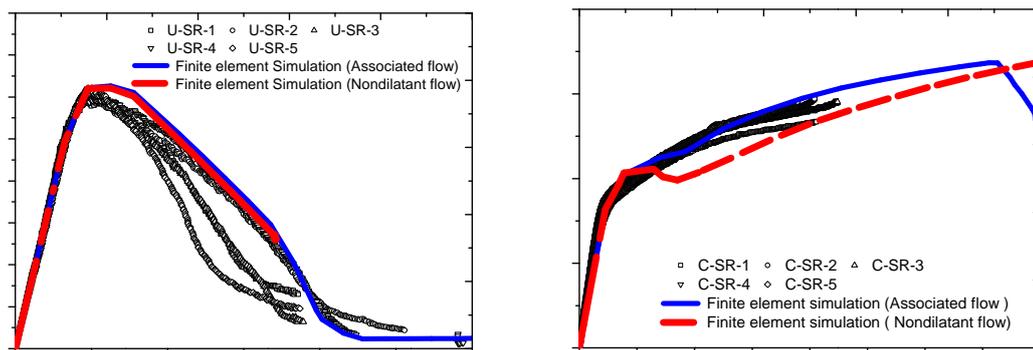
Figure (6): Principal plastic strain of unit cell at failure

5. VALIDATIONS

The unconfined steel reinforced resin compressive tests were simulated numerically using solid element C3D8R[20] see Fig.7. The uniaxial true stress and strain relationship and material parameters of the linear Drucker-Prager model are based on the multiscale simulation. The nominal stress-strain relationship of unconfined steel reinforced resin comparisons between finite element simulation and experimental results is shown in Fig. 8. A good agreement is observed. Finite element model of the confined resin experiments was built to validate the efficiency of the linear Drucker-Prager model when predicting resin behaviour with confinement. The nominal stress-strain of confined resin comparisons between finite element simulation and experimental results is shown in Fig. 8. A good agreement is observed, indicating the Drucker-Prager model could effectively model the confined condition of the resin. The fracture initiation strain at the peak load from “nondilatant flow” model is a little larger than if the “associated flow” model is used.



(a) Unconfined (b) Confined
Figure (7): Finite element model of steel reinforced resin tests



(a) Unconfined (b) Confined
Figure (8): Predicted stress-strain relationship and experimental results of steel reinforced resin specimens

6 CONCLUSION

- The friction angle β , the ratio of the yield stress in triaxial tension to the yield stress in triaxial compression K, and the dilation angle ψ of the linear Drucker-Prager plastic model is obtained based on numerical homogenization to efficiently consider the confinement effects on steel reinforced resin. For associated flow hardening, the friction angle is 12.16° and 49.80° , the ratio K is 0.92 and 0.78, and the dilation angle ψ is 12.16° and 49.80° respectively for resin and steel reinforced resin. For non-dilatant flow, the friction angle is 49.80° and 52.04° , the ratio K is 1.00 and 1.00, and the dilation angle ψ is 0.0° and 0.0° respectively for resin and steel reinforced resin.

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Evaluation of Stress Intensity Factors in Cracked Plates and Shells Using Irwin's Integral and High-order XFEM

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ABSTRACT

This paper presents a novel framework based on Irwin's integral for evaluation of stress intensity factors (SIFs) in cracked plates and shells, using the extended finite element method (XFEM) with high order enrichment terms. The mixed interpolation of tensorial components (MITC) plate element based on the Mindlin-Reissner theory is used and enriched with discontinuous and high-order near tip functions. Irwin's integral is first reformulated for plates and shells and then evaluated using enriched degrees of freedom in XFEM. In this way, SIFs can be obtained in a closed-form and thus no special post-processing is needed. The accuracy of the formulation is studied on several benchmark examples of cracked plates. We consider an inclined crack problem with structured and unstructured quadrilateral meshes, and two cracks approaching each other. In both cases the method shows good accuracy and in particular the latter case shows the advantage of this method over the classical J-integral method. Finally, we demonstrate excellent performance on a shell problem of a cylinder with a circumferential crack subject to tension or torsion.

An Adaptive Galerkin Finite Element Method for Forced Vibration of Skeletal Structures in Structural Engineering

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ABSTRACT

As an advanced means of finite element method (FEM), the adaptive finite element method (AFEM) has been deeply studied and widely used in mechanics and engineering ever since it was proposed in 1980s. The basic idea of adaptivity is that, the user pre-specifies an error tolerance instead of a well-designed mesh in conventional FEM, the algorithm itself adjusts and generates an adaptive mesh, and finally a solution satisfying the error tolerance in certain norm is obtained. Actually the present research originates from the adaptive solution of one-dimensional steady convection-diffusion problem, for which the conventional Bubnov-Galerkin FEM may produce a bad result because of numerical oscillation, as we all known. Based on the Energy Element Projection (EEP) method for super-convergence computation of both the function and its derivatives in the post-processing stage of FEM, an efficient adaptive Galerkin FEM was established for boundary-value problems (BVPs) of ordinary differential equations (ODEs). And then it was extended to the adaptive solution of initial-value problems (IVPs) of ODEs, which in structural engineering are usually resulted from the finite element discretization of dynamic problems. The Galerkin weak form for IVPs and the adaptive strategy using EEP super-convergent solutions to estimate errors and guide the mesh refinement will be presented firstly. The forced vibration of skeletal structures, which is fundamental in structural dynamics, is a time- and space-dependent problem of partial differential equations (PDEs) in mathematics. Discretizing the structure along the axial direction of members with the conventional FEM, a system of IVPs is obtained and then solved with the adaptive strategy mentioned above, i.e. the adaptive analysis of time domain is realized. After that, the similar strategy is implemented to the axial coordinate of the members, i.e. the adaptive analysis of space domain is realized as well. As a result, an optimal time-space mesh and the corresponding dynamic solution with satisfying accuracy are obtained. The basic idea and the implementation algorithm of this adaptive Galerkin FEM for time- and space-dependent problems will be elaborated secondly. Several representative examples including Euler or Timoshenko beams and the plane frame under harmonic loads or seismic loads will be given to demonstrate the efficiency of the method finally. This work is part of the project supported by the National Natural Science Foundation of China (No. 51508305).

A Scaled Boundary Finite Element Based Node-to-Node Scheme for Three Dimensional Frictional Contact Problems

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ABSTRACT

A new node-to-node scheme is proposed for three dimensional frictional contact analysis involving large sliding, with the aid of the scaled boundary finite element method. Treatment of non-matching contact interface which may result from different meshes of contact bodies or large tangential slippage remains to be one of the key obstacles in contact mechanics. Methods based on the finite element method often fail the patch test and/or require a complicated implementation, especially in three dimensional problems [1]. Moreover, initial penetrations and gaps introduced by non-matching meshes in curved contact interface may cause difficulty in contact pair identification and hence affect solution convergence. In the proposed method, non-matching meshes are treated using polyhedral elements constructed in the scaled boundary finite element method. The polyhedral elements may have an arbitrary number of faces. Only the boundary of a polyhedral element is discretised thereby providing highly flexibility in mesh transition [2]. Non-matching meshes can be easily converted to matching ones with a surface remeshing procedure which inserts nodes along the contact interface. The method allows the use of the simple and robust node-to-node contact analysis algorithm. The initial penetrations and gaps can also be eliminated. The surface remeshing procedure is limited to the contact interface only and no volume remeshing is required in the scaled boundary finite element method. The contact constraint is formulated and solved directly as a mathematical programming problem known as a mixed complementarity problem. Contact constraints of non-penetration and stick slide condition are described directly in a complementarity format. The constraints are strictly satisfied without having to resort to user-specified control parameters. The irreversibility of friction is accommodated in a rate formulation that is solved in a sufficiently accurate stepwise fashion. Through numerical examples, it is demonstrated that the proposed method not only can pass the patch test but also is stable and accurate, especially in conjunction with higher order elements. References: [1] V. A. Yastrebov, Numerical Methods in Contact Mechanics, John Wiley & Sons, 2013. [2] E. T. Ooi, C. Song, F. Tin-Loi, A scaled boundary polygon formulation for elasto-plastic analyses, Computer Methods in Applied Mechanics and Engineering 268 (2014) 905-937.

Numerical Simulation of Damage Effects of a Carbon Fiber Composite Cylinder Subjected to Laser Irradiation and Axial Compression

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ABSTRACT

The specific aim of this study is to investigate damage effects of the carbon fiber composite subjected to compression load and laser irradiation simultaneously. The intense laser irradiation can lead to ablation and damage of materials. Because the damage effects of composites irradiated by laser are very complex, only the thermal decomposition and oxidation reaction are taken into account in our study. The ALE adaptive grid method and a UMESHMOTION subroutine in ABAQUS are applied to simulate the ablation progress. The three-dimensional ablation evolution of a carbon fiber composite cylindrical shell is obtained and the influence of the related parameters on the critical buckling load is discussed as well.

Predicting Dislocation-Interface Reactions from the Atomistic to the Microscale

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ABSTRACT

The dislocation-interface reaction in materials is inherently multiscale since both the atomic structure of the interfaces and the long-range fields of the dislocation pile-up at the interface come into play. In this work, we present a concurrent atomistic-continuum (CAC) method for multiscale modeling and simulations of dislocation-interfaces interactions. The interfaces to be investigated include twin boundaries in bi-crystalline metallic materials, phase boundaries in amorphous/crystalline and crystalline/crystalline multilayered metallic composites. The CAC method is based on a finite element implementation of a multiscale formulation in which the reconfiguration of crystal structures and slip systems in crystalline solids are embedded. CAC models of typical material systems, such as bi-crystalline Cu and Al with twin boundaries, multilayered $\text{Cu}_x\text{Zr}_{1-x}/\text{Cu}$, and fcc/bcc/fcc composites, are constructed. With a fully atomistic resolution at the interface and coarse-grained atomistic resolution in the regions away from interfaces, CAC models require significantly less computational cost than that by fully atomistic simulation. Most importantly, the atomistic natures of dislocation nucleation, migration, and interactions are preserved in the coarse region away from the atomic-scale interfaces. CAC simulations reveal main mechanisms underlying dislocation-interface interactions from the atomic to the microscale. In bi-crystalline Cu and Al specimens, the dislocation-twin boundary reaction is found to always follow the recombination-redissociation process, without forming any twin boundary dislocations in process of recombination. In $\text{Cu}_x\text{Zr}_{1-x}/\text{Cu}$, with the dislocations being "piled-up" at the amorphous/crystalline interfaces, strong local stress concentrations near the amorphous-crystalline interface lead to the devitrifications in amorphous layers. In contrast, in fcc/bcc/fcc nanolaminates, dislocation pile-ups at the fcc/bcc interface is found to assist phase transformation from bcc to fcc. Our results elucidate the discrepancies between atomistic simulations and experimental observations of dislocation-interface reactions and highlight the importance of directly modeling dislocation-interfaces interactions using concurrent multiscale models.

Modeling and Simulation of Nonequilibrium Complex Flows

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ABSTRACT

Nonequilibrium complex flows are ubiquitous in nature and play an important role in both the engineering fields and our daily lives. The existing various interfaces, complex forcing and relaxation processes results in very complicated hydrodynamic and thermodynamic responses. It is known that a Navier-Stokes(NS) model is not sufficient to capture the complicated non-equilibrium behaviors, and the spatial and temporal scales which the microscopic molecular dynamics simulation can access are too small to be comparable with experiments. The Monte Carlo simulation has a similar constraint on the system size and evolution time. Under such cases, a kinetic model based on the Boltzmann equation is more preferable. In this talk, we will briefly review the progress of discrete Boltzmann modeling, simulation and analysis of nonequilibrium complex flows in our group in recent years. The topics are relevant to multiphase flows, shock waves, combustions and hydrodynamic instabilities. Mathematically, the only difference of discrete Boltzmann from the traditional hydrodynamic modeling is that the NS equations are replaced by a discrete Boltzmann equation. But physically, besides the macroscopic behaviors described by the NS model, the discrete Boltzmann model(DBM) presents more kinetic information on the Thermodynamic Non-Equilibrium (TNE). Via the DBM, it is convenient to perform simulations on systems with flexible Knudsen number. The observations on TNE have been used to estimate the deviation amplitude from thermal equilibrium state, to recover the main feature of real distribution function, to distinguish different stages of phase transition, to discriminate and capture various interfaces, etc. References [1] A. Xu, C. Lin, G. Zhang, Y. Li, Multiple-relaxation-time lattice Boltzmann kinetic model for combustion, *Physical Review E* 91, 043306 (2015). [2] Y. Gan, A. Xu*, G. Zhang, S. Succi, Discrete boltzmann modeling of multiphase flows: hydrodynamic and thermodynamic non-equilibrium effects, *Soft Matter* 11, 5336 (2015). [3] H. Lai, A. Xu*, G. Zhang, Y. Gan, Y. Ying, S. Succi, Nonequilibrium thermohydrodynamic effects on the Rayleigh-Taylor instability in compressible flows, *Physical Review E* 94, 023106 (2016).

Atomistic Modeling and Simulations on Mechanics and Thermal Transport of Heterostructures.

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ABSTRACT

Heterostructures that are assembled by interfacing two-dimensional (2D) materials in an either lateral or vertical manner offer a unique platform for future energy efficient and multifunctional nanoelectronics. Unfortunately, the inherent difference of material lattice structures between layer components or external loading conditions will render mechanical deformation in heterostructures. The mechanical deformation could easily alter phonon activities by coupling with atom vibration, and thus changes thermal properties of heterostructures. Given the feature thickness (one to several atomic) of heterostructures, the thermal properties, which play an important role in thermal management of various electronic and thermal devices, are critical for maintaining optimal functionality of these devices, and yet is far less investigated due to their couplings with mechanical deformation. Understanding the fundamental thermal transport of heterostructures under mechanical deformation will be crucial for designing emerging heterostructures of relevance to applications in stretchable electronic and thermal devices with controllable heat-power dissipation and thermal management. In the present study, we develop atomistic modeling and simulation techniques to probe the effect of mechanical deformation on thermal transports in both vertical and lateral heterostructures, and to design heterostructures with mechanically controllable thermal properties. The fundamental thermal transport mechanism of both vertical and lateral heterostructures under various mechanical deformation are elucidated with the help of atomistic simulations. Further, guided by atomistic simulations, we present several proof-of-concept designs of heterostructures and demonstrate their mechanically tunable performance.

Resonant Attenuation of Stress Wave in a Particulate Composite

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ABSTRACT

Efficient wave attenuation is crucial for the protection of strong shock wave. In this presentation, a numerical study of resonant attenuation of stress wave in a particulate composite is performed using Finite Element Method (FEM). Coated particles, which are embedded in an elastic matrix, play roles of resonance units. Each unit consists of a core of high density and a soft interface, and it works like a mass-spring oscillator. Local resonance occurs when the natural frequency of the particle matches the frequency of incident wave. For a given incident wave, by designing the corresponding natural frequency of the coated particles, the local resonance is stimulated. Thus, a maximum amount of the incident energy transforms to the kinetic energy of the particles, leading to significant wave attenuation during the propagation in the composite. In this study, the effects of particle size and material properties on the natural frequency are also investigated.

SPH Simulation of Water Spray Generated by Aircraft Chine-Tire on the Contaminated Runway

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ABSTRACT

The spray produced by aircraft tire running on contaminated runway may enter the inlet of engines, and lead to the compressor stall, surge, or even combustor flameout. Scholars used to study this problem by full-scale aircraft spray test, which may cost a lot, and get only a little valid data. According to the analysis of the interaction between tire and water, the numerical models of an elastic chined tire rolling in the water are established by coupled smoothed particle hydrodynamics (SPH) and finite element method (FEM). Then, the mechanism of the chine effect on the water spray is studied and the shape of chine is analyzed to avoid the potential danger. However, from the full-scale tests, we found that the chine tires could effectively suppress the spray at lower taxiing speed of aircraft, while it would suddenly lose effectiveness at higher speed. In order to discover the problem, we tried several steps. (1) A falling test of aircraft tire is constructed to investigate the suppression effect of the chine. The influence of the chine height is discussed in detail. (2) To reveal the reduction of suppression effect at high taxiing speed, several factors of the chine geometry, the water depth and the taxiing speed are considered. A quantitatively study is performed to analyze the inhibitory effect with respect to the hydroplaning speed of an aircraft tire and the height of chine. The results shows that when the height of chine exceeds a certain value, very small increment may cause significant ineffectiveness to suppress the water spray. (3) Based on the above understandings, a new configuration of aircraft chine-tire is proposed, which would be effective at a wide range of taxiing speed.

Strongly-coupled Direct Numerical Simulation of Thermal Turbulence in Channel with Rib-tabulator and Surface-roughness

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ABSTRACT

Abstract - The paper applied the state-of-the-art flow numerical simulation method, i.e. Direct Numerical Simulation (DNS), and strongly coupled the DNS with the heat-transfer governing equation to solve the thermal-turbulence phenomena in a cooling channel with rib-tabulator of turbine-blade, see Ref [1]. In order to capture the turbulent thermal-fluid phenomena in reality and subsequently to build more accurate flow and heat-transfer models, three innovative approaches were applied to the studies. On the computational side, the current research developed a highly efficient and reliable parallel solution technology based on the Flexible-cycle Additive-correction Multi-grid method (Ref [2]). The surface roughness of the cooling vane was considered by including the roughness geometry in the DNS and an innovative Immersed-Boundary (IB) method, see Ref [3], was applied to handle the geometry complexities due to the existence of surface-roughness. On the flow physics side, the time-sequencing fully-developed turbulent inflow conditions were generated through a temporal DNS of turbulence in a channel, which permitted to accurately resolve the fully-developed thermal turbulence problem in the cooling vane with rib and surface roughness structures in the modern aero-engine. The computational results were expected to provide a variety of advantages over the conventional Reynolds-averaged Navier-Stokes (RANS) approach, including the more accurate mean flow field and the heat-transfer performance predictions. The results presented the typical wall-turbulence characteristics, such as the near-wall coherent structures for a regular smoothed wall and more interesting flow structures caused by a wall roughness as well as their effects on the heat transfer properties. The strongly-coupled flow and heat-transfer simulation captured the temperature and its derivative fields, exhibiting the attractive coherent streaky patterns associated with the turbulence. These research will advance the current knowledge of the surface-roughness on the flow field and heat transfer. References [1] J.C. Han, Recent Studies in Turbine Blade Cooling, International Journal of Rotating Machinery, 10(6): 443–457, 2004. [2] H. Xu, W. Yuan, M. Khalid, Design of a high-performance unsteady Navier-Stokes solver using flexible-cycle additive-correction multi-grid technique. Journal of Computational Physics, 209: 504–540, 2005. [3] H. Xu, Developing LES/DNS Simulation Capability based on Immersed Boundary Method coupled with FCAC Multigrid and AMR Techniques, The 18th International Conference on Finite Elements in Flow Problem, Taipei, 2015.

Mechanical Integrity and Electrical Behaviors of Lithium-ion Pouch Cells under Dynamic Mechanical Loadings

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ABSTRACT

Dynamic mechanical loading is one of the major catastrophic factors that trigger short-circuit, thermal runaway, or even fire/explosion consequences of lithium-ion batteries (LIBs). In this study, the mechanical integrity and electrical coupling behaviors of lithium-ion pouch cells under dynamical loading were investigated. Two types of experiments, namely compression and drop weight tests, were designed. The state-of-charge (SOC) and strain rate (or impact energy in drop weight tests) dependencies of batteries, as well as their coupling effect, were examined. Furthermore, the electrical performance of battery was investigated through real-time monitoring of voltage change during loading. Experiments on LiCoO₂ lithium-ion pouch cells show that the increase in SOC or strain rates may increase battery structure stiffness. In addition, strain rate may intensify battery structure stiffening with the SOC effect. Experiments show that open-circuit voltage of battery has a relationship with compression deformation. The gradient of voltage drop increases with strain rates, thereby leading to changes in failure mode and rapid deterioration of batteries. Results may provide useful insights into the fundamental understanding of electrical and mechanical coupled integrity of LIBs and lay a solid basis for their crash safety design.

A Novel High-order Time Integration Method for Structural Dynamics

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ABSTRACT

A novel high-order time integration method for structural dynamic analysis is proposed. The main idea of the proposed method is to implement an error estimation and recovery based on the weak form Galerkin method. By implementing the recovery scheme, displacement, velocity and acceleration with fourth order accuracy can be calculated, which is more accurate than the common algorithms with second order accuracy such as the Newmark method. Examples of a SDOF, a Multi-DOF system and a frame structure are given to verify the accuracy of the proposed method. Simple numerical tests show a significant reduction in the computation time for the proposed method in comparison to that for the Newmark method.

Mesh Refinement Strategies Based Multiscale Isogeometric Optimization of Lattice Material

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ABSTRACT

This paper presents a new approach to design the structures made of heterogeneous lattice structured material. The optimization problem is formulated as minimizing the macroscopic structural compliance under a prescribed material volume constraint while accounting for microstructures of the lattice material. This approach is based on isogeometric analysis(IGA) method and bidirectional evolutionary structural optimization(BESO) technique. IGA is adopted for computing stiffness matrix and nodal displacements of elements on macro-scale. The elements on micro-scale is obtained by mesh refinement strategies of IGA and the effective mechanical properties of microscopic elements is calculated by IGA and asymptotic homogenization(AH). To concurrently optimize the topology of structure and topology of elements on micro-scale, BESO is used as the optimization algorithm. Solutions of numerical tests show that the mesh refinement strategy based isogeometric optimization scheme can address the nonlinearity two-scales problem.

Effect of Twin Boundary on the Deformation Behaviors of Magnesium Nanopillars: A Molecular Dynamics Study

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ABSTRACT

The plasticity of magnesium and its alloys, which causes the limited formability and restricts the wide application, is currently an active field of research. Deformation twinning plays a crucial role in hexagonal close-packed metals, because it can change the crystal orientation and accommodate the plastic deformation. In this work, deformation behaviors of magnesium nanopillar with two different modes of twin boundaries (TBs) during uniaxial tension and compression were investigated using molecular dynamics simulations. The effect of TB density on the mechanical behaviors and related mechanisms were considered. Simulation results showed strong asymmetry mechanical properties between tension and compression for both TB modes. Furthermore, it found that enough number of {10-11} TBs has the potential to make the flow stress increases with strain in a rather smooth manner. References [1] H. Somekawa, A. Singh, C. A. Schuh, Effect of twin boundaries on indentation behavior of magnesium alloys, *Journal of Alloys and Compounds* 685 (2016) 1016–1023. [2] Q. Yu, L. Qi, K. Chen, R. K. Mishra, J. Li, A. M. Minor, The nanostructured origin of deformation twinning, *Nano Letters* 12 (2012) 887–892. [3] M. Pozuelo, S. Mathaudhu, S. Kim, B. Li, W. Kao, J.-M. Yang, Nanotwins in nanocrystalline MgAl alloys: an insight from high-resolution TEM and molecular dynamics simulation, *Philosophical Magazine Letters* 93 (2013) 640–647.

Mesoscale Modeling of Dislocations in Face-Centered Cubic Metals

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ABSTRACT

The motions of dislocations, linear crystalline defects with cores that are nanometers wide, control the plastic deformation of metallic crystals. While atomistic simulations are desirable in studying dislocations, they are limited to nano/submicron length scale even with dedicated high-performance computing resources. On the other hand, classical continuum models do not naturally incorporate the discrete atomic-scale degrees of freedom and other evolving internal state variables needed to define the dislocation core structure. Since their inception in the early 1990s, atomistic/continuum coupling approaches have been developed to combine the atomistic domain (for short-range dislocation core) with the continuum domain (for addressing long-range dislocation elastic fields). By employing coarse-grained or reduced order models in regions away from those requiring short-range accuracy, these methods can simulate problems at the micron-scale that is not accessible to typical fully-resolved atomistics. In this work, we explore the core structure/energy/stress of dislocations in face-centered cubic metals using the concurrent atomistic-continuum (CAC) method [1]. Employing the underlying interatomic potential as the only constitutive relation, CAC admits a two-way exchange of displacement discontinuities through a lattice between atomistic and coarse-grained domains. As a result, it is more accurate than one-way linking multiscale strategies. In this talk, results of CAC simulations are compared against fully resolved atomistics, as well as two other meso-scale dislocation models, i.e., phase-field dislocation dynamics [2] and atomistic phase-field microelasticity [3]. The generalized stacking fault energy surface is calculated using density functional theory and employed within the phase field model. Possible sources of differences among these mesoscale calculations are discussed. The issues of core energy double counting in phase field methods and grid/mesh sensitivity are explored. Two atomic-level stress formulations are employed and compared. A dislocation loop is then modelled using all three mesoscale approaches to shed light on their abilities to describe more realistic mixed-type configurations, potentially assisting in designing stronger metallic materials. References: [1] Shuozhi Xu, Rui Che, Liming Xiong, Youping Chen, David L. McDowell, A quasistatic implementation of the concurrent atomistic-continuum method for FCC crystals, *Int. J. Plast.* 72 (2015) 91-126 [2] Irene J. Beyerlein, Abigail Hunter, Understanding dislocation mechanics at the mesoscale using phase field dislocation dynamics, *Phil. Trans. R. Soc. A* 374 (2016) 20150166 [3] Jaber R. Mianroodi, Bob Svendsen, Atomistically determined phase-field modeling of dislocation dissociation, stacking fault formation, dislocation slip, and reactions in fcc systems, *J. Mech. Phys. Solids* 77 (2015) 109-122

Investigation of High-pressure Induced Densification of Silicate-based Glasses Using Atomistically-informed Peridynamic Model

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ABSTRACT

An atomistically-informed peridynamic model is proposed for the study of high-pressure induced densification of silica glass. Start by employing a molecular dynamic(MD) model of amorphous silica(a-SiO₂), which is described by enforcing Tersoff potential on the continuous random network of SiO₂. Constitutive relations, as well as densification mechanism are thoroughly investigated within the MD framework. It's shown that the results obtained from MD simulation are in good agreement with available experimental data. Based on the results from MD simulation, a constitutive model that accounts for the anomalous densification behavior is proposed and next reformulated to a state-based peridynamic model. We argue that the peridynamic model is capable of reproducing coarse-scale quantities of interest from MD simulation and yet being able to simulate at component level. Numerical simulations of the atomistically-informed peridynamic model are carried out and validated against the results from MD simulation.

Multimaterial Topology Optimization of Thermoelectric Devices

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ABSTRACT

Since it is not feasible to achieve high efficiency of the thermoelectric generator (TEG) consisting of only one single thermoelectric material in a wide temperature range, this paper proposes a novel methodology based on topology optimization for finding the optimal geometry of a TEG made of multiple materials. The conversion efficiency of the TEG is formulated as the objective to be optimized. The proposed method is implemented using the Solid Isotropic Material with Penalization (SIMP) method. Simple relationships are established between the density function of SIMP and the corresponding physical properties of thermoelectric materials within each temperature sub-interval. This method can maximize the potential of different thermoelectric materials by distributing each material into its optimal working temperature range. Several numerical examples are provided to demonstrate the validity of the proposed method and some comparisons between the single-material TEG are given as well.

Research on Curing Deformation of Thermosetting Resin Matrix Composites During Autoclave Forming

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ABSTRACT

During autoclave processing, the thermal expansion of composites, chemical shrinkage of resin as well as the interaction with the mold can result into shape distortion in composites structures, which has a very negative factor on the performance of composite products. In this paper, the cure kinetics reaction of prepreg system was firstly investigated, then the temperature and degree of cure during curing process were predicted by means of ABAQUS. Moreover, a thermodynamics and mesomechanics constitutive model was developed to study the curing deformation with numerical simulation method, in which the properties of density, special heat capacity, thermal expansion and thermal conductivity coefficients varies with the temperature and curing degree. The time varying characteristic of these parameters were measured with the instruments of differential scanning calorimetry (DSC), dilatometry (DIL) and laser flash apparatus (LFA), respectively. Further, the influence of layup and processing parameters on curing deformation was studied by finite element analysis. Acknowledgements This work is supported by National Key Research and Development Program of China (2017YFB1102800), Shaanxi international science and technology cooperation and exchange program (2016KW-057) and Seed Foundation of Innovation and Creation for Graduate Students in Northwestern Polytechnical University.

On the Gradient of Lode's Angle

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ABSTRACT

One of most important ways to model the complex behaviors of loading-path dependent geomaterials within the framework of plasticity theory is construct the yield criterion and/or the plastic potential as functions of stress invariants, including Lode's angle. Consequently, the gradient of Lode's angle with respect to stress tensor plays an essential role both in elasto-plastic constitutive equations and in the finite element analysis. From the theoretic and computation perspectives, the first-order gradient of the plastic potential with respect to stress tensor is indispensable in the orthogonal flow rule, while that of the yield criterion is used to impose the consistency condition, and the second-order gradient of plastic potential is required in computing local Jacobi matrix to guarantee the second-order convergence rate in Newton-Raphson iteration. The formulas of the gradient of Lode's angle in literatures were highly nonlinear and cumbersome. Moreover, they became singular when the stress state happened to be an axisymmetric one. The objective of this study is to derive the simple and concise formulas for the first- and second-order gradient of Lode's angle with respect to the stress tensor in principal stress space, respectively. The formulas have completeness and can be expressed explicitly. Numerical examples show that the resulted formulas simplify the calculation of plastic flow direction, plastic strain tensor, and local Jacobi matrix. They render the return-mapping algorithm more efficient for FE analysis with complex elasto-plastic constitutive relations. Furthermore, we proposed a new perturbation scheme that enables the perturbation error of the first-order gradient tensor of Lode's angle to be evaluated when a stress state is axisymmetric. Finally, some important properties of our findings are also provided.

Orthotropic A-FEM for Static Strength Prediction in Composite Laminates

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ABSTRACT

Typical composites exhibit complex, multiple fatigue damage events that are strongly coupled and developed in a stochastic microstructure. The gradual progression of such damages is of primary concern for safety and tolerance design of composite structures. Those traditional methods based on linear elastic fracture mechanics are not effective and efficient for such complex damage processes. In order to accurately assess/predict the composite fatigue life, it is necessary to explicitly account for the progressive evolution of all major types of discrete damage events with high fidelity. In this paper, we extended a recently developed augmented finite element method (AFEM) that can accurately and efficiently account arbitrary cracking in isotropic materials to deal with the much more complicated multiple fracture problems in composites. A composite laminate may develop multiple types of cracks (matrix cracking, fiber rupture in tension/kinking in compression, and delamination) at different locations depending on the in-situ stress environments. Moreover, these modes of damages are not isolated in most of the practical application, i.e. intra-ply transverse cracking will lead to inter-ply delamination and delamination propagation may lead effect fiber damage. Also, typical composite exhibits complex asymmetric mechanical behaviors between tension- and compression-dominant stress state. Strong nonlinearity in shear stress-strain is also critically important for delamination crack growth. Therefore in our A-FEM formulation, we adopt the mechanism-based Sun's criteria for crack initiation under general in-situ stress states. Upon satisfaction of a certain criteria, i.e., matrix tension/compression/shear crack, fiber tension rupture crack, fiber-compression kink band formation, a cohesive crack will be initiated within an element. The element will be augmented into two subdomains connected by a specified mixed-mode cohesive law of the initiated crack type. The elemental equilibrium of this augmented problem will be solved using a newly developed consistency-check based algorithm, which has been proven to have mathematical exactness for piece-wise linear cohesive laws. A rigorous verification and validation process will be presented to demonstrate that the developed orthotropic A-FE can initiate and propagate various types of cracks under different stress environments, and can predict the entire (linear or nonlinear) stress-strain curves all the way to two-part failure for any quasi-static laminates tension tests. Further, we shall demonstrate that, this element can be used together with any cohesive interface elements to account for the important damage coupling between ply cracking and interlaminar delamination.

An Active Compliant Micro-assembly Control Method Based on Micro-force Sensing

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ABSTRACT

This paper studies the spatial nondestructive assembly problem of vulnerable micro-parts, and presents an active compliant assembly control method based on micro-force. By analyzing the various contact states of vulnerable micro-parts, the relationship model between the output of six-dimensional micro-force sensor and position-pose error of peg-in-hole micro-assembly is established. Specifically, a method to solve the uncertainty of contact state based on active constraint state is presented. This method makes the relationship between the position-pose error of peg-in-hole and the force condition of micro-parts corresponded to each other, therefore, the position-pose error of peg-in-hole can be estimated by micro-force and micro torque. Furthermore, an automatic control method based on two dimensional micro-forces and two dimensional micro torques is proposed to solve the coupling problem between multi-dimensional forces and position, multi-dimensional torques and pose angle. Especially for the peg-in-hole micro-assembly task with initial position-pose deviation, the experimental results verify the effectiveness of the proposed method. Finally, the interference fit of peg-in-hole micro-assembly is also analyzed, and the experimental results verify the active compliant micro-assembly control method can be applied as well. The solution of these problems will avoid the micro-assembly jammed, which is beneficial to the nondestructive assembly of the vulnerable micro-parts and has important application significance. Keywords: micro-assembly, micro force, position-pose control, interference fit, compliant control

Dynamic Analysis of Crack Problems by SFBEM Based on Erdogan's Solutions

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ABSTRACT

The appearance of cracks on engineering structures has large influence on the structural dynamic characteristics. The Erdogan's solutions for static analysis of an infinite cracked plate are introduced in this paper. Based on the above fundamental solutions, mathematical formulation and computational implementation of the spline fictitious boundary element method (SFBEM) are presented for dynamic analysis of linear-elastic cracked plates, in which the stress boundary conditions on the crack surface are automatically satisfied and the singular behaviour at the crack tip can be naturally captured. The eigenvalues and mode shapes of cracked plates can be obtained using the proposed method. The dynamic stress intensity factors and structural responses of cracked plates can also be achieved with the present approach. Numerical examples are given to demonstrate that the proposed method is superior to the traditional finite element method (FEM) in terms of accuracy and efficiency.

THE OPTIMIZATION ANALYSIS OF THE VIBRATION CHARACTERISTICS OF A BUS FRAME

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Keywords: Adams, Workbench, deceleration zone, simulation analysis

Summary: *In this paper, Adams and Workbench simulation software are used to explore the vibration characteristics of a passenger car when driving through the deceleration belt with different loads. The vibration frequency of the bus-body is taken as an evaluation index, when the passenger car passes through the deceleration belt. By comparing the excitation frequency and the natural frequency of the body frame in the suspension system, When the frequency values are close, the resonance phenomenon is easy to occur, and the dangerous position of the body frame is determined. Finally, by improving the structure of the dangerous parts, the vibration characteristics of the body are optimized and the resonance phenomenon is avoided.*

1 INTRUCTION

With the improvement of people's living standard, private cars are also gradually increasing, However, people's demand for the comfort of the car is getting higher and higher, and the comfort of the car is mainly related to the vibration of the body and the noise environment in the car. At the same time, the rapid development of automobile manufacturing industry is devoted to the development of high performance, economic and comfortable products. Abnormal vibration can affect the life, safety and reliability of the vehicle when the car passes some special road surface.

In this paper, the passenger car driving simulation analysis is carried out under the special traffic speed, vehicle vibration characteristics, in order to further study the road condition to provide theoretical basis for the influence of body structure, and for better optimization of body structure provides the certain reference value.

The author has published two papers on this subject, and on this basis^[1,2], further research has been done.

2 THE ESTABLISHMENT AND ANAL SIS OF THE SIMULATION MODEL OF DECELERATION BELT

2.1 The simulation model of deceleration belt is established

In this paper, the wheel diameter of the simulation model is 0.64 m, and according to the relevant provisions of JT/T713-2008 rubber speed belt standard^[3].The simulation model of deceleration belt is selected, whose width is $a=0.32$ m, and the height is $h=0.05$ m.

Then run the road file in Adams/View software to see the speed bump model, as shown in figure 2-1^[4].

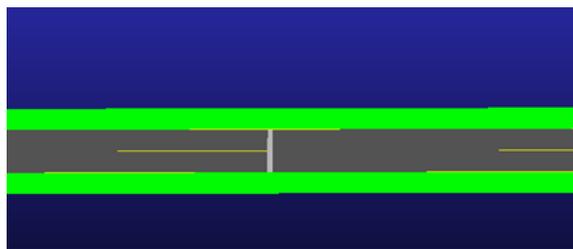


Fig. 2-1 The model of road deceleration

2.2 The simulation experiment of speed reduction belt pavement is carried out

The final simulation model of vehicle model and road surface model is determined in Adams/View analysis module^[5-7], as shown in fig.2-2. When the passenger trains at different speed and different loads to drive through the deceleration belt, the simulation test of the ride

smoothness is carried out, and the vibration frequency of the body in the vertical direction acceleration is output.

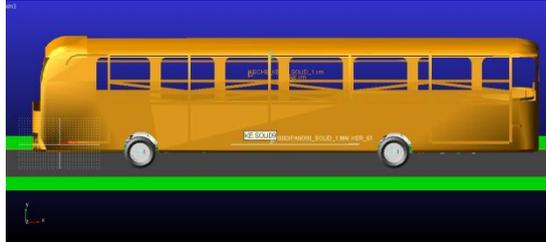
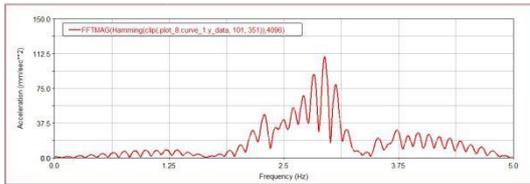


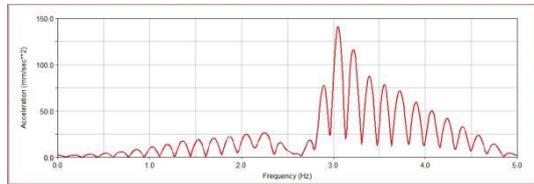
Fig. 2-2 the simulation model of the bus passing the speed bump

The speed of the bus is set at 15km/h, 20km/h, 25km/h, 30km/h. When the passenger car is in no-load, medium and full load, it outputs the vibration of the body in the vertical direction. The simulation results are as follows, See figure 2.3-2.4:

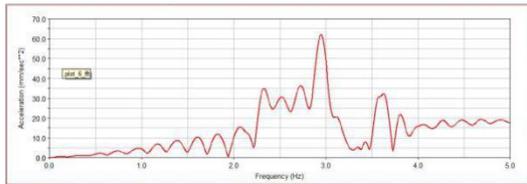
(1) When the bus was empty, driving at different speeds ,the simulation results are shown in figure 2.3 :



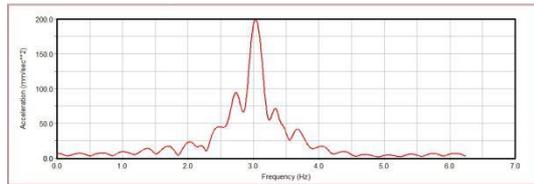
(a) The driving speed is 15km/h



(b) The driving speed is 20km/h



(c) The driving speed is 25km/h



(d) The driving speed is 30km/h

Fig. 2-4 The simulation results under different speeds at no-load

(2) When the bus is with medium load, driving at different speeds, the simulation results are shown in figure 2.4:

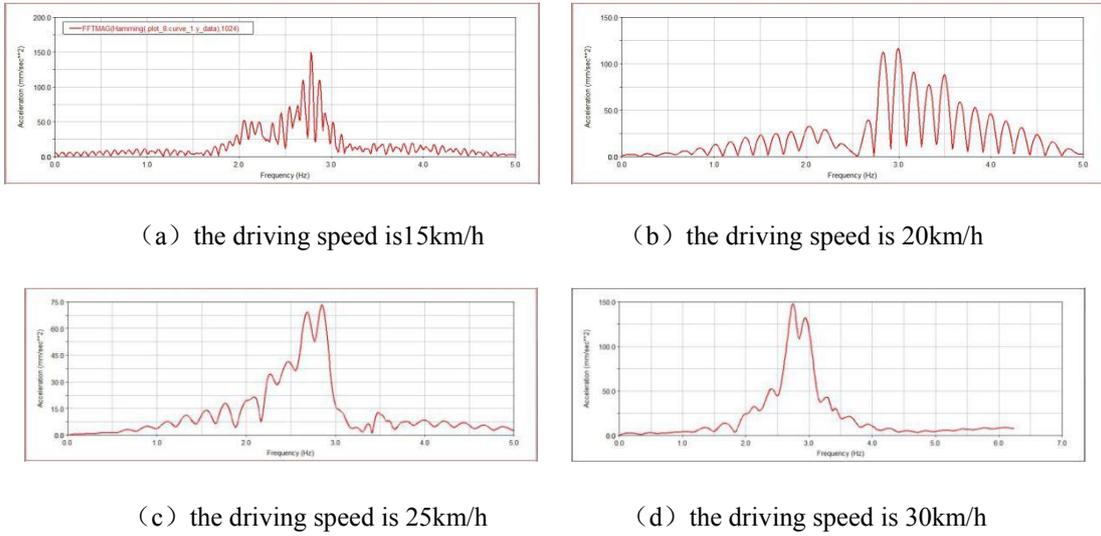


Fig. 2-4 The simulation results under different speeds at half-load

(3) When the bus is with full load, driving at different speeds, the simulation results are shown in figure 2.5:

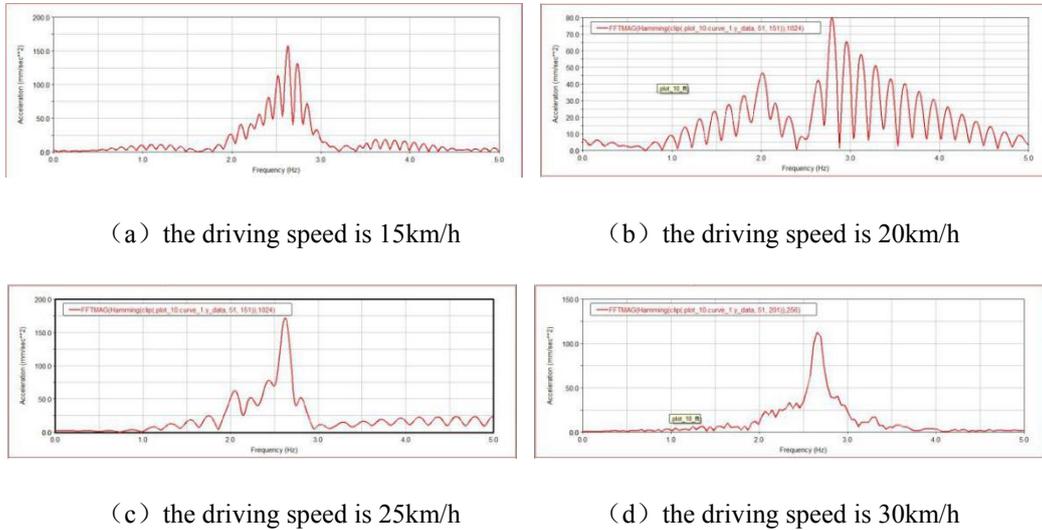


Fig. 2-5 The simulation results under different speeds at full load

The above simulation results are calculated, as shown in table 2-1:

Tab 2-1 The results of simulation

Load \ Speed	Speed			
	15km/h	20km/h	25km/h	30km/h
Full load	2.6 (Hz)	2.8 (Hz)	2.7 (Hz)	2.6 (Hz)
Middle load	2.8 (Hz)	3.0 (Hz)	2.9 (Hz)	2.8 (Hz)
No load	2.9 (Hz)	3.1 (Hz)	2.9 (Hz)	3.0 (Hz)

The experimental results show that the vibration frequency of the maximum acceleration of the body in the vertical direction is the evaluation index, and the acceleration of the vertical direction is significantly increased when the bus passes the speed bump. When the vibration acceleration of the body is the maximum, the corresponding vibration frequency of the vehicle is the vibration frequency of the passenger car.

When the bus is traveling at a speed of 15km/h- 30km/h, the frequency range of the body is 2.6-3.1Hz.

3 MODAL ANALYSIS OF BOD SKELETON

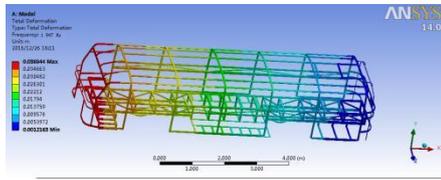
Using PRO/E software to build body frame model, import the finite element analysis software Workbench to conduct modal analysis. Main parameters are defined: the elastic modulus is 2.1×10^{11} , poisson ratio is 0.3, and the density is 7800kg/m^3 [8,9]. A finite element model is obtained for the mesh partition of the body frame model, as shown in fig.3-1^[10].



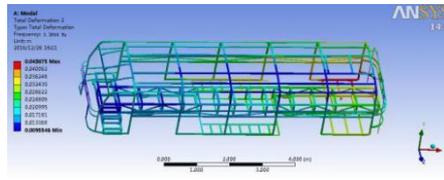
Fig. 3-1 Finite element model of bus body

3.1 Analysis of the results

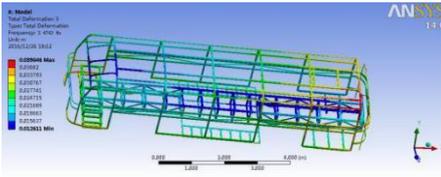
This paper mainly studies the low-frequency characteristics of the body frame, so in the simulation test, only the first six order natural frequencies and corresponding modes of vibration are recorded. Before the optimization of the body structure, finite element analysis of the body skeleton was carried out, and the vibration patterns were obtained, as shown in fig.3-2



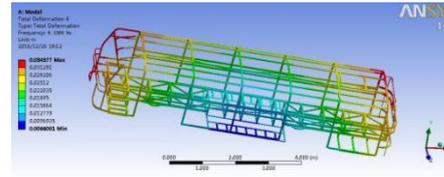
The first order vibration graph



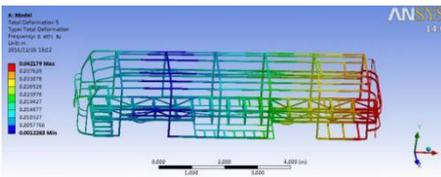
The second order vibration graph



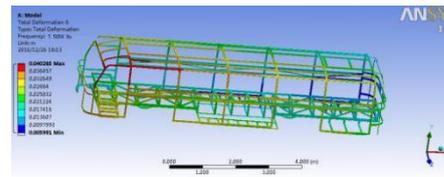
The third order vibration graph



The fourth order vibration graph



The fifth order vibration graph



The sixth order vibration graph

Fig. 3-2 The front of the body is a six-order modal mode

The intrinsic frequency of the vehicle body skeleton modal analysis is shown in table 3-1.

Tab 3-1 Natural frequency of body frame

Order	Frequency (Hz)	The main characteristics
1	2.868	The front part of the car bends longitudinally
2	3.384	Local deformation at the end of the car
3	3.474	Local deformation of front and rear
4	6.109	Heavy deformation of the front and rear
5	6.497	The small deformation of the locomotive and the large deformation of the car
6	7.506	Integral mode and local mode mixing

Comparing the natural frequency with the excitation frequency, the comparison curves are drawn, as shown in figure 3-3

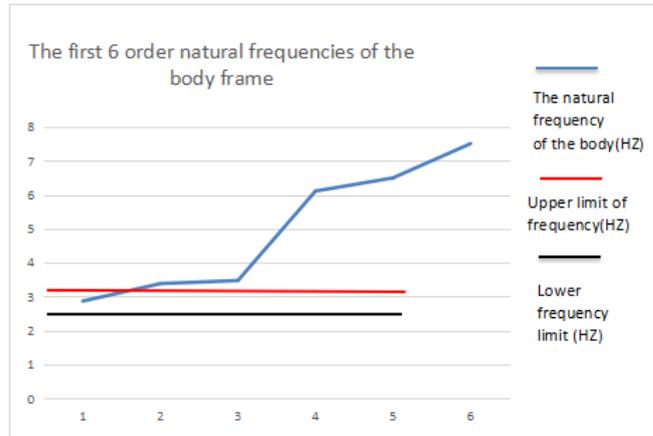


Fig. 3-3 Analysis of simulation results

The vibration frequency range of the body in vibration system is 2.6-3.1 Hz by Adams software. Comparison of modal analysis results can be obtained: The first order natural frequency of the body frame is 2.868 Hz, The first order natural frequency of the body frame is 2.868 Hz, In the range of vibration frequency of the vehicle during the deceleration zone ,By analyzing the mode of vibration, it can be concluded that the head position is easy to be resonant.

3.2 Local improvement of bus body structure

By comparing the results of two simulations, the resonant frequency was obtained, and the resonant position of the body was determined by the corresponding mode of vibration, then The improved position of body frame structure is determined. In order to not affect the life and performance of the body structure during the design process and meet the structural strength and stiffness requirements of the body,Therefore, local improvement of body frame structure is carried out.

3.2.1 Structural improvement method

In the case of not making too much change in the structure of the body frame, the area of resonance in the frame structure is optimized. Thus, the final structure improvement method is determined. Main content is: Based on the mode diagram, the resonance location is determined, then change the regional body frame structure geometry size in China, or to increase or decrease of beam, and then analyzed many experiments on the points adjustment, which change the inherent characteristics of body structure, and finally determine the improvement plan. Then, change the geometrical dimensions of the body skeleton structure in the region, or increase or decrease the number of beams. The optimal improvement scheme is finally obtained through several test and analysis.

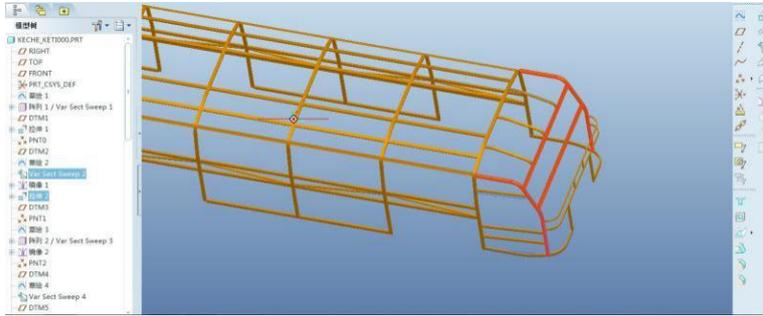


Fig. 3-4 The position of structure improved

The specific improvement parameters are: four square steel pipes of the front position, and the thickness of steel tube δ is changed from 1mm to 2mm. See figure 3-5.

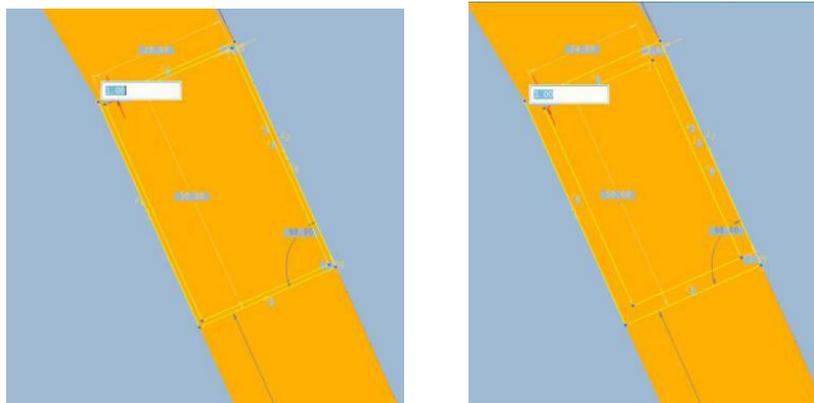
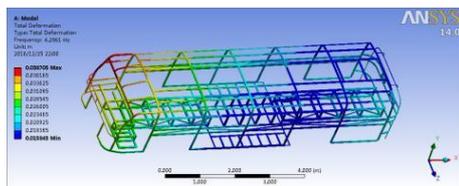


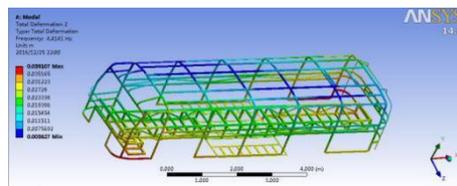
Fig. 3-5 The measurement of structure improved

3.2.2 Finite element analysis after modification

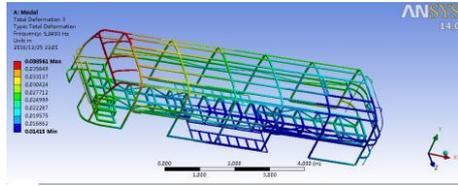
The modal analysis of the locally modified body skeleton model is carried out again. The grid is divided according to the size of the cell, and the modal analysis is performed after the grid division. The modal diagram is shown in Fig. 3-6.



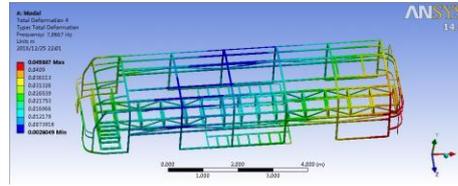
The first order vibration graph



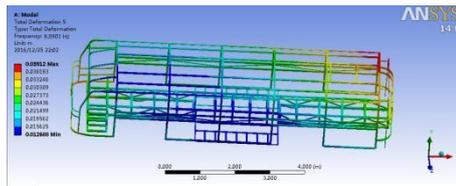
The second order vibration graph



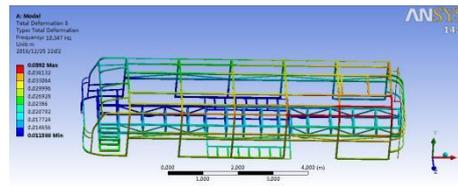
The third order vibration graph



The fourth order vibration graph



The fifth order vibration graph



The sixth order vibration graph

Fig. 3-6 The first six order modal shapes of the body after structural improvement

After the structural improvement, the natural frequency of the bus body skeleton modal analysis is shown in table 3-2

Tab 3-2 Natural frequency of structure improvement

Order	frequency (Hz)	The main characteristics
1	4.296	Front position X-axis distortion
2	4.414	Integral mode and local mode mixing
3	5.9493	Local deformation of the front part
4	7.9867	Local deformation of front and rear
5	8.9903	Local deformation of locomotive
6	10.347	Integral mode and local mode mixing

4 MPARING OF RESULTS BEFORE AND AFTER OPTIMI ATION

The natural frequency comparison chart of each order before and after the improvement of the frame structure of the body is drawn, as shown in fig.4-1.

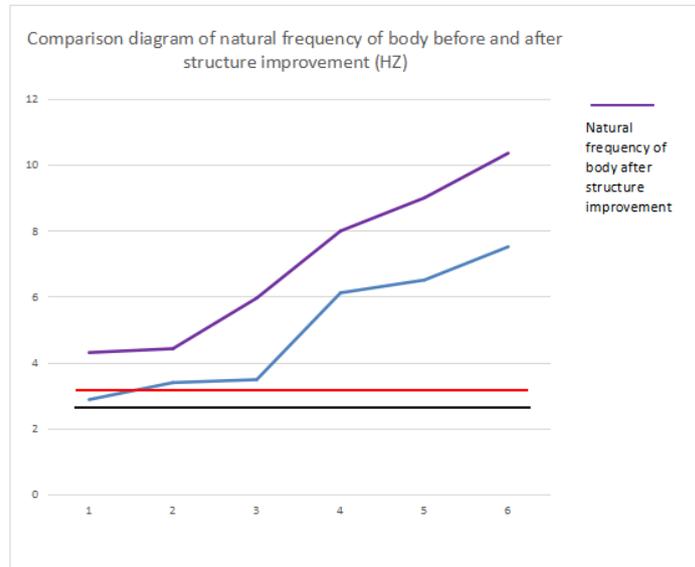


Fig. 4-1 Analysis of simulation results

After structure optimization, body frame of each order natural frequency significantly deviate from the body in the process of driving vibration frequency range, especially prone to the first order natural frequency of resonance, effectively avoid the possibility of resonance body and suspension system.

CONCLUSION

- (1) The vertical vibration frequency range of the passenger car is 2.6-3.1Hz with the speed of 15km/h-30km/h and different loads.
- (2) When the coach is driving through the deceleration zone, there will be a resonant phenomenon in the position of the bus head
- (3) The inherent frequency of the body is obviously deviated from the resonant frequency range, so the resonance phenomenon can be avoided effectively.

ACKNOWLEDGEMENTS

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Flux Flow along a Grain Boundary within a High Temperature Superconductor: A Molecular Dynamics Simulation

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ABSTRACT

Abstract: With the rapid development of high-temperature superconductors, it is of great importance to understand the precise current density and flux distribution around grain boundaries (GBs) of superconducting materials. In this paper, we simulate the flux dynamics by the molecular dynamics method. All the flux lines and pin centers are regarded as point particles, whereas those along the GB are different with the ones in grains. An extra force is added on the flux lines within the width of a GB to reflect the anisotropy of the potential function between flux lines and pin centers around the GB. Details of flux flow along the GB are displayed in this work, and the critical forces and the I-V curve are obtained. The simulated results, as well as a theoretical model [1] we proposed, are discussed in this paper which can be helpful for understanding the underlying mechanism of critical current density of polycrystalline superconductors. Key words: superconducting film, molecular dynamics method, grain boundary. REFERENCE [1] F. Xue, Y. Gu, and X. Gou, J. Supercond. Nov. Magn. 29, 2711 (2016).

A Fully Eulerian Finite Element Approach to Predicting Largely Deforming and Phase Changing Solids

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ABSTRACT

Problems with severe solid deformations or even phase-changes are ubiquitous in many applications in engineering and sciences alike. Typical ones might be liquefaction and re-consolidation of granular continua as observed in earthquakes and landslides. Traditionally, the continuum mechanics perspective of solids has followed the Lagrangian paradigm, where the governing equations are posed for a fixed material point. Contrastingly, for fluids the governing equations are posed for a fixed spatial point, which is also referred to as the Eulerian reference frame. The contrast between Lagrangian vs Eulerian formulation of solids and fluids stems from the nature of different constitutive relations. The approaches to solve for solids and fluids problems are hence dichotomous. This brings trouble when solids and fluids coexist and need to be simulated simultaneously with good efficiency. The proposed approach is to formulate the problem, regardless of the state of the material being fluid or solid, using an Eulerian frame of reference. The primary variable is taken as the inverse of the deformation mapping to a reference configuration similarly to [1]. By noting that the material derivative of the reference coordinates along a fixed particle is actually zero, one may recover the inverse mapping by solving an additional advection equation. With the inverse mapping at hand, both the total deformation for solid constituents as well as rates of deformation for fluid constituents may be obtained. Some recent efforts have been invested in this area and some of the relevant work can be found in [1, 2]. To handle the evolving free surface, we propose to introduce an order parameter advected along the deformation of the solid. Additional fields, such as the phase field of fracture mechanics, as well as internal state variables for inelastic materials are also advected along the flow. We will develop higher order Discontinuous Galerkin methods in order to solve the resulting system of governing equations. Sample problems will showcase the capabilities of the proposed method in relation to state-of-the-practice tools. References: [1] K. Kamrin, C. H. Rycroft, and J.-C. Nave. "Reference map technique for finite-strain elasticity and fluid solid interaction". In: *Journal of the Mechanics and Physics of Solids* 60.11 (2012), pp. 1952-1969. [2] D. I. W. Levin, J. Litven, G. L. Jones, S. Sueda, and D. K. Pai. "Eulerian solid simulation with contact". In: *ACM Transactions on Graphics* 30.4 (2011), p. 1.

A 3D h-Adaptive Methodology for Simulating Metal Forming Processes with Crack Initiation and Propagation Using a Hexa-tetra Based Multi Level Remeshing Technique

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ABSTRACT

We propose an h-adaptive 3D FE methodology in an explicit solver to represent the initiation and propagation of cracks in ductile materials in which cracks are represented as locations of all the fully damaged elements [1]. The size of the loading sequence is adapted to control both the size and the number of the damaged elements to be deleted. An elasto-plastic model fully coupled with damage is used [2]. Size indicators based on plasticity, damage and their dissipation are proposed. The goal is to refine the mesh in active areas as well as coarsen the mesh in inactive areas. An original multi deformable octree technique is proposed in order to adapt (refine and coarsen) the tetrahedron mesh with robustness and efficiency, at a reduce computational cost. No unstructured mesh generator is used nor local remeshing technique. A first coarse hexahedral mesh is created and each element is thereafter considered as an octree which can be deformed throughout the simulation. The remeshing process is purely analytical based on octree refinement or coarsening. Once all octrees have been created, a tetrahedron mesh is created in each octant with conforming meshes at the interface between octrees. After a loading step, the mesh is deformed and the newly created octrees are reconstructed while taking into account the structure deformation. Issues to reduce numerical diffusion and to preserve peak value which may occur during the transfer of variables are discussed and a hybrid transfer operator based on enhanced diffuse approximation is presented [3]. Solutions based on surface subdivision are proposed to smooth the crack along inactive areas and enable contact. [1] Yang, F.T., Rassineux, A., Labergere, C., Saanouni, K., A 3D h-adaptive local remeshing technique for simulating the initiation and propagation of cracks in ductile materials (2018) Computer Methods in Applied Mechanics and Engineering, 330, pp. 102-122. [2] Saanouni, K., 2013. Damage mechanics in metal forming: Advanced modeling and numerical simulation. John Wiley & Sons. [3] Yang, F.T., Rassineux, A., Labergere, C., A hybrid Meshless-FEM field transfer technique minimizing numerical diffusion and preserving extreme values: Application to ductile crack simulation, Finite Elements in Analysis & Design, in press, 2018.

A New Model for Fiber Bridging in Cementitious Composites Based on Large Deflection Beam Theory

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*The Hong Kong University of Science and Technology, **The Hong Kong University of Science and Technology

ABSTRACT

The behavior of Engineered Cementitious Composites (ECC) is strongly affected by the relationship between total fiber bridging stress and crack opening width. In order to extract this relationship, the single fiber pull-out behavior is usually studied first. From experimental data, when a fiber inclined to the crack surface is pulled along the direction perpendicular to the crack, the peak pull-out load is commonly observed to increase with the inclination angle. This is often explained in terms of the snubbing effect for flexible strings passing over a frictional pulley, but such an explanation is not satisfactory because the bending stiffness of the fiber used in ECC is not negligible. In this study, a new model for fiber bridging is proposed. The fiber on each side of the crack is treated as a continuously supported beam lying on the elastic foundation (which represents the matrix) plus a free length protruded into the crack. The protruded part is treated as a cantilever supported at its end by an equivalent spring group representing the part of fiber inside the matrix. The relationship between bridging stress and crack opening width is then calculated by the combination of pulling, bending as well as shearing. Since the protruded part is very likely to undergo large deflection, large deflection theory of bending is applied. From the simulation results on PVA fibers, although fiber's slip-hardening effect and the frictional pulley at the fiber exiting matrix point are not taken into account, bridging stress can still exhibit the increasing trend with the inclination angle. The shear deflection can also be proven to be unimportant compared to fiber's bending, thus this model gives a new physical explanation to the empirical snubbing effect as the consequence of increasing bending forces. In addition, other two models based on small deflection are also developed. Through the comparison with large deflection model, it turns out consideration of both bending stiffness provided by axial force and large deflection is necessary. The effects of different parameters such as embedded length and fiber/matrix stiffness ratio are then studied, and it is found that the ratio of inclined fiber's maximum pullout force to the corresponding aligned fiber's maximum pullout force increases with the fiber/matrix stiffness ratio and decreases with increasing embedded length.

Deterioration of Atomistic Mechanisms That Bind Mutated Type IV Collagens with Integrin

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ABSTRACT

Human type IV collagen constitutes a major component of extracellular scaffolds for the assembly and mechanical stability of certain types of tissues, especially that of glomerular basement membranes. Type IV collagen is also a vital component for interacting with cells, which is crucial for cell adhesion and differentiation. Approximately 80% of Alport Syndrome cases are caused by mutations in the COL4A5 gene encoding the $\alpha 5$ chain of type IV collagen. The effect of Gly missense mutation within and adjacent to the predicted integrin binding sequence on collagen-integrin binding was investigated by combining atomistic molecular simulations and recombinant collagen experiments. The introduction of any reported Gly substitution in Alport syndrome (Gly - Glu, Gly - Val and Gly - Asp) in the recombinant collagen abolished its integrin binding affinity, even if the mutation site was not located within the essential integrin binding site. To probe this phenomenon in detail on a molecular level, the atomistic mechanisms of the binding process were analyzed with atomistic molecular dynamics simulations. The integrin-binding domain of each wild-type and mutant model collagen-like peptide were constructed and structurally aligned to the experimentally determined crystal structure of type I collagen bound to integrin&amp;amp;apos;s $\alpha 2$ inserted (I)-domain (PDB: 1DZI). These bound structures were then refined through replica exchange simulations with solute tempering in explicit solvent. Similarly, the integrin $\alpha 1$ I-domain (PDB: 1PT6) was modelled and refined through structural alignment with the integrin $\alpha 2$ I-domain to create a second set of collagen-integrin complexes. Through this approach, we will be able to determine the hydrogen-bonding topology, structural and conformational changes in the collagens and integrins, as well as quantitatively measure the binding free energy through enhanced sampling with methods such as adaptive biasing force.

Topology Optimization of Particle-matrix Composites for Optimal Fracture Resistance

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^{****}Hunan University, Changsha, China

ABSTRACT

We propose a topology optimization framework for optimizing the fracture resistance of two-phase composites through a redistribution of the inclusion phases [1,2]. A phase field method [3] for fracture capable initiation, propagation and interactions of complex microcracks networks is adopted. This formulation avoids the burden of remeshing problems during crack propagation and is well adapted to topology optimization purpose. An efficient design sensitivity analysis is performed by using the adjoint method, and the optimization problem is solved by an extended bi-directional evolutionary structural optimization (BESO) method. The sensitivity formulation accounts for the whole fracturing process involving cracks nucleation, propagation and interaction, either from the interfaces and then through the solid phases, or the opposite. The spatial distribution of material phases are optimally designed using the extended BESO method to improve the fractural resistance. We demonstrate through several examples that the fracture resistance of the composite can be significantly increased at constant volume fraction of inclusions by the topology optimization process. References [1] L. Xia, D. Da, J. Yvonnet, Topology optimization for maximizing the fracture resistance of quasi-brittle composites, *Computer Methods in Applied Mechanics and Engineering*, 2018, in press. [2] D. Da, J. Yvonnet, L. Xia, G. Li, Topology optimization of particle-matrix composites for optimal fracture resistance taking into account interfacial damage, submitted. [3] B. Bourdin, G. A. Francfort, J. J. Marigo, The variational approach to fracture, *Journal of elasticity* 91 (1-3) (2008) 5–148.

Multi-Time Scale Simulations of Coupled Transient Electro-Mechanical Fields for Modeling Finite Strain Piezoelectricity

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ABSTRACT

Abstract: This paper presents the wavelet transformation based multi-time scaling algorithm for finite element simulations of piezoelectric materials in finite strain theory. The free energy for piezoelectric materials in finite deformation is derived through a consistent thermodynamic framework, from which the constitutive equations for the mechanical stress, Maxwell stress and electrical displacement are formulated in terms of strain and electric fields. A fully coupled total Lagrangian finite element formulation is devised for rigorously modeling piezoelectric materials with highly nonlinear constitutive laws and time dependent material effects. One major challenge in computational modeling of many piezoelectric devices including actuator and sensor structures is the large discrepancies in the frequencies of electrical signal and mechanical vibrations and this requires simulating a large number of cycles with electric excitation time period for reaching to a state of mechanical deformation in the time domain. The conventional single time-scale integration schemes are constrained by the stability and convergence requirements of the highest frequency response and therefore are insufficient to advance with the changes in the low frequency field. The present work addresses these issues by developing the wavelet transformation based multi-time scaling (WATMUS) algorithm for dynamic piezoelectric simulations in the finite element framework [1,2,3]. The wavelet transformation projects the high frequency (fine time scale) electric potential and its first time derivative, displacement and velocity fields through translation and dilation of an appropriate set of scaling functions on the low frequency (coarse time scale) response with monotonic evolution. The method significantly enhances the computational efficiency in comparison with conventional single time scale integration methods. The performance of the WATMUS method is demonstrated by several examples proving its accuracy and efficiency for solving nonlinear coupled systems. References: [1] Yaghmaie, R. and Guo, S. and Ghosh, S. (2016). "Wavelet transformation induced multi-time scaling (WATMUS) model for coupled transient electro-magnetic and structural dynamics finite element analysis." *Comput. Methods Appl. Mech. Eng.* 303, 341–373, <https://doi.org/10.1016/j.cma.2016.01.016>. [2] Yaghmaie, R. and Ghosh, S. (2017). "Multi-time scaling based modeling of transient electro-magnetic fields in vibrating media with antenna applications." *Comput. Mech.* 60 (1), 117–141, <https://doi.org/10.1007/s00466-017-1396-1>. [3] Yaghmaie, R. and Ghosh, S. (Submitted). "A computational model coupling transient electro-mechanical fields for analyzing finite deformation piezoelectric material behavior"

Development of Multi-Stage Failure Simulation Using the Principle of Hybrid-type Virtual Work

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ABSTRACT

ABSTRACT Multi Stage Failure Simulation (MSFS) is a simulation that seamlessly analyzes various destruction states of structures. We propose an explicit dynamic model to solve sequentially large deformation behavior as MFSF. In order to realize MSFS, we focus on the following two points. (1) Determine of mechanism, (2) Analysis on the rigid body motion after the collapse. In this proposal, we use the Hybrid-type Penalty Method (HPM) [1] suitable for MSFS. In this method for calculating the displacement field, it is assumed that an independent linear displacement field for the axial direction and an independent displacement field for the bending of each element are combined. The continuity conditions of displacement are incorporated by using a penalty function. The elastic solution obtained with this method is consistent with the exact solution. Moreover, the approach of the dynamic model after collapse is similar to the Distinct Element Method (DEM), it is possible to explain the behavior of the failure mechanism after the formation [2] [3]. In this paper, we include the similar mechanism judgment method of structural stability in this algorithm. Possibility of applying MSFS in various collapse patterns is proposed by this. The effectiveness of the proposed method is demonstrated by the simple numerical examples. REFERENCES [1] K. Yamaguchi and N. Takeuchi, Discrete Limit Analysis for Framed Structures by using Hybrid-type Penalty Method, Bulletin of Research Center for Computing and Multimedia Studies, Hosei University, 30, 2016. [2] T. Yagi, N. Takeuchi, K. Yamamura, and M. Kusabuka, An explicit dynamic method for a discrete element model using the principle of hybrid-type virtual work, Proceedings of the 11th World Congress on Computational Mechanics, Barcelona, Spain, 2014. [3] T. Yagi and N. Takeuchi, An explicit dynamic method of Rigid Bodies-Spring Model, International Journal of Computational Method, 12, 1540014, 2015.

Application of Hamiltonian Flows to Exploring Parameters of Mathematical Models in Situations with Insufficient Data

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ABSTRACT

Although parameter estimation is essential in mathematical modeling of phenomena in the real world, enough number of data is not necessarily available because experiments are often labor intensive or require expensive equipment. In these cases, the problem of parameter estimation often yields an underdetermined least squares problem, and optimal parameters in the models are not determined uniquely. To choose an appropriate set of parameters, it is necessary to enumerate qualitatively different sets of parameters. To facilitate this problem, we propose an application of Hamiltonian flows to explore the set of optimal solutions. In our algorithm, a set of optimal parameters is first assumed to be obtained by, e.g., a quasi-Newton method. Then a set of optimal parameters are explored by following the Hamiltonian flows of which the energy function is defined by using the objective function. Because the Hamilton equation preserves the energy, all points on the orbits are optimal solutions if the initial conditions are imposed by using an optimal solution.

Comparison between numerical approaches to simulate a supersonic nozzle

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ABSTRACT

The supersonic separator is a new compact and efficient technology for CO₂ separation from Natural Gas with high CO₂ fraction. It consists of a supersonic nozzle with a swirling flow. The cooling caused by the expansion of the flow leads to condensation of the CO₂, which then moves to the outer portions of the nozzle due to centrifugal effects, where it can be collected. As a preliminary step on a comprehensive study of this complex device, we compare the use of different computational fluid dynamics (CFD) packages for the simplified problem of a supersonic divergent-convergent nozzle, both in terms of accuracy and of computational cost for the same number of degrees of freedom. The codes we consider are: Ansys Fluent, a widely-used commercial software based on finite volume methods; SU2, an open-source suite of tools for performing CFD simulations and optimization, also based on finite volume methods; Nektar++, an open-source high-order spectral/hp element framework, which includes a compressible flow solver using the Discontinuous Galerkin method; and a least square solver implemented using the FEniCS project, which is an open-source finite element computing platform. The simulation results of a planar nozzle with the same area distribution and pressure ratio as Arina (2004) are presented and compared with experimental data. References: Renzo Arina 2004, Numerical simulation of near-critical fluids. Applied Numerical Mathematics, 51 (4), 409-426.

Method of Manufactured Solutions in Large Deformation Problems of Hyperelasticity

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ABSTRACT

In recent years, numerical simulations have been contributed to crucial decision making in the various fields such as medical engineering. Then we need to give the information on the credibility of modeling and numerical simulations to the public. Verification and validation are attracting great attention as a framework to provide such information on modeling and simulations. In this work, we apply the method of manufactured solution (MMS), which is a technique of verification proposed by Roache[1] for fluid dynamics, to nonlinear problems of solid mechanics. In the conventional method of manufactured solution, spatial derivatives of stresses derived from given solutions are required to calculate body forces. Such derivatives can hardly be evaluated in problems of nonlinear materials and hence it has not been popular in solid mechanics. The author developed an alternative technique to calculate equivalent nodal vectors associated with 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 and finite element discretization. The actual procedure to calculate equivalent nodal force vectors is similar to the evaluation of internal force in the standard 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 hyperelasticity, which is often used to describe rubber-like materials. In the method of manufactured solutions, an arbitrary displacement field can be prescribed formally. However incompressible or nearly incompressible properties need to be considered in the large deformation problems of hyperelasticity and manufactured solutions that ignore such properties may lead to physically unreasonable external loads or numerical instabilities. Thus we developed a procedure to construct displacement fields in which volumetric changes are controlled in the large deformation state. [1] P. J. Roache and S. Steinberg: Symbolic manipulation and computational fluid dynamics," AIAA Journal, Vol. 22, No. 10, pp. 1390-1394, 1998. [2] T. Yamada: Verification Procedure Based on Method of Nearby Problems for Finite Element Analysis of Solid, ASME 2015 Verification and Validation Symposium, 2015.

Optimum Design of Microstructures Considering Wave Dispersion Using the High Order Homogenization Method

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ABSTRACT

The wave dispersion is a phenomenon appearing in heterogeneous media, by which waves with different wavelengths propagate with different velocities [1]. These effects are modeled by an additional fourth-order term (namely Burnett coefficient) in the homogenized wave equation. Considering the dispersion phenomenon is important in industrial applications, since the periodic size of the microstructures is finite. To begin with, this presentation shows optimum design of microstructures considering wave dispersion [2]. Additionally, the high order homogenized wave equation with an obtained optimal solution is computed using the first Fourier transform Method. References [1] F. Santosa, W. W. Symes, A Dispersive Effective Medium for Wave Propagation in Periodic Composites, SIAM Journal on Applied Mathematics, 1991, Vol.51, pp.984–1005. [2] G. Allaire, T. Yamada, Optimization of dispersive coefficients in the homogenization of the wave equation in periodic structures, HAL Id: hal-01341082.

Interfacial Fracture of Surface Coating under Impact Loading Produced by Pulsed Laser Irradiation

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ABSTRACT

This study aims to evaluate coating adhesion, i.e. the interfacial strength of coatings and thin films by using pulsed-laser irradiation technique. This method uses strong ultrasonic wave induced by pulsed laser irradiation, such that interfacial fracture of coating occurs due to strong wave. For this irradiation, grease layer is applied to the back of the substrate and a pulsed laser is irradiated, so that ablation occurs in grease layer, inducing strong elastic wave. The elastic wave propagates from the back surface of substrate to the coating surface, and tensile stress acts on the coating/substrate interface. Since such pulsed laser irradiations cause the coating delamination and spallation, this technique is also called laser spallation method. In parallel, the out of plane displacement is measured by using a laser ultrasonic interferometer (continuous wave CW laser). First, to determine critical laser energy of interfacial fracture, pulsed laser irradiation is conducted with various levels of irradiation laser energy. The delamination can be detected from the observation of coating surface morphology and out-of-plane displacement waveform. This study evaluates adhesion of various coating, such as the oxide film on carbon steel substrate and electroplated coatings etc. Furthermore, computation of elastic wave propagation using FDTD (Finite difference time domain) and FEM (Finite Element Method) are carried out to estimate tensile stress developed at the coating film/substrate interface. Based on the above results, the interfacial strength is estimated quantitatively. In addition, the durability of interfacial adhesion is investigated by repeated laser irradiation with similar manner of the above (laser spallation method). In other words, we try to investigate cyclic fatigue of interfacial fracture. In this test, repetitive lower stress loading is applied to the interface using repeated laser irradiations. It is found that repetitive loading encourages interfacial fracture, whose stress level is lower than that of single (monotonic) laser irradiation (of above laser spallation method). Upon various levels of irradiation laser energy, interfacial adhesion durability is investigated. In parallel, numerical simulation (FDTD and FEM) is conducted to estimate interfacial stress for delamination. This result may be useful for adhesion durability, when a coating/film is used under cyclic loading in long time period. Reference: Quantitative evaluation of adhesion quality of surface coating by using pulse laser-induced ultrasonic waves, Surface and Coatings Technology, Vol.286(2016) pp.231-238 Measurement of interfacial fracture toughness of surface coatings using pulsed-laser-induced ultrasonic waves, Journal of Nondestructive Evaluation, Vol.37,2 (2018) pp.1-11]

Development of Hyperelastic Analysis Using Meshfree Particle Method

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ABSTRACT

Development of Hyperelastic Analysis using Meshfree Particle Method Nobuki Yamagata¹, Masakazu Ichimiya¹, Noritaka Matsuoka² and Pedro V. Marcal³ 1 Advanced Creative Technology Co., Ltd., 2 Sumitomo Riko Company Limited, 3 MPACT Corp. Key Words: MeshFree Particle Method, SSPH, Hyperelastic Material, Large Deformation. The large deformation analysis approaches using finite element method (FEM) to simulate the incompressible and the nearly incompressible behavior of hyperelastic materials such as rubber have been carried out to handle the mesh distortions and the volumetric locking resulting from the incompressibility constraint. And on the other hand, in order to solve large deformation problem of solid materials, the SPH method is used which is a kind of particle method based on the meshfree Lagrangian scheme. This method can handle the governing equations and existing constitutive models for structural analysis problems and can solve large deformation problems without mesh distortion. However, this conventional SPH method has disadvantages of impossibility to apply to static and thermal stress analyses in the solid mechanics. To remove these disadvantages, other meshfree methods have been proposed such as Corrected Smoothed Particle Method (CSPM), Reproducing Kernel Particle Method (RKPM), Symmetric Smoothed Particle Hydrodynamics Method (SSPH) and so on. The SSPH method has an advantage over any other meshfree methods because the basic functions have continuous capabilities of derivatives up to the expected order. In this study, using the Improved SPH method (SSPH) the nonlinear formulation for the large deformation analysis of rubber materials, which are considered to be hyperelastic and nearly incompressible, is presented. In a same manner as FEM, the behaviour of rubber is classified as hyperelastic in which the strain energy density function can be defined in this study. The choice of reference configuration influences the kinematics, constitutive law, and SSPH formulation. The original configuration is selected as the reference configuration in the SSPH calculation. The second Piola-Kirchhoff stress and Green-Lagrangian strain are used as the stress and strain measures, respectively. Several numerical examples are presented to study the characteristics of SSPH and to demonstrate the effectiveness of this method in large deformation analyses of hyperelastic materials. And it is also demonstrated that this method has a superior performance to the conventional finite element methods in dealing with large material distortions.

Solid-liquid Coupled Material Point Method for 3-D Simulations of Soil Deformation and Flow

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ABSTRACT

A new solid-liquid coupled material point method is developed to accurately predict a collapse process of ground structures such as slopes and embankments subjected to excess pore pressure during a heavy rainfall, which involves a transition process from a soil structure to flowing mixture. The governing equations are formulated based on Biot's two-phase mixture theory and separate sets of Lagrangian material points are used to discretize unknown variables of solid and liquid phases in reference to the literature [1][2]. The material behavior of solid phase is represented by the Drucker-Prager's type plastic flow model combined with Hencky's hyperelasticity, whereas the liquid is assumed to be a Newtonian fluid. To improve the accuracy, robustness and efficiency in comparison with the previous studies, the incompressibility is assumed for not only solid grains, but also pore liquids, which necessitates the continuity equation of the liquid phase. By applying the Chorin's projection method to the momentum equation of the liquid phase, pore water pressure can be obtained as a solution of Poisson equation. For the discretization in space, we employ B-spline basis functions [3], which suppress numerical oscillations when a material point crosses the mesh boundary. Since MPM does not require us to search for adjacent particles, the computing costs are significantly small, the proposed method is also suitable for parallel computing with an appropriate domain decomposition so that large-scale 3-D simulations would be possible. Several numerical examples are presented to demonstrate the capability of the proposed method that inherits the beneficial features of MPM. A collapse analysis of an embankment with water inflow boundary conditions is a typical example problem to incorporate the performance, by which the superiority in computational efficiency over existing approaches can be confirmed. References [1] Bandara, S., Soga, K., Coupling of soil deformation and pore fluid flow using material point method. *Computers and Geotechnics*, 63, 2015, pp. 199–214. [2] Bui, H. H., Nguyen, G. D., A coupled fluid-solid SPH approach to modelling flow through deformable porous media. *Internat. J. Solids Struct.*, 125, 2017, pp. 244–264. [3] Steffen, M., Kirby, R. M., Berzins, M., Analysis and reduction of quadrature errors in the material point method (MPM). *Internat. J. Numer. Method Engrg.*, 76(6), 2008, pp. 922–948.

Advanced Multi-Physics CFD Simulations for Engineering Problems

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ABSTRACT

Computational Fluid Dynamics (CFD) has been completely matured in the engineering sense. Nowadays, we can use CFD for research and development of various machines. However, most targets of current CFD are limited to single-phase flows. Thus, in near future, we have to focus on multi-phase flows which are typically of multi-scale and multi-physics. Based on this consideration, I have been tackling the modeling and simulations of multi-physics engineering problems such as ice accretion, particle deposition and sand erosion in a jet engine. In these problems, the flow fields strongly depend on surface deformation. For example, ice layer whose thickness is few mm is formed on fan blades of a jet engine in icing environments. Such a thin ice layer can lead to 10% performance degradation. Therefore, exact reproduction of surface deformation is critical in the simulations. At first, I adopted a finite difference method (i.e. grid-based method) because of my long experience. Using a finite difference method, I and my students succeeded in simulating the temporal changes of flow field, wall surface and machine performance due to icing, deposition and erosion. However, in the simulations, we had to smooth the wall surface so that we could re-generate the grid along the deformed or rough surface. This might reduce or destroy the accuracy of simulations. (It is too difficult to verify and validate this point.) So, I decided to change the strategy, and introduced a particle-based method, since it does not need any grid system. It should be noted that a particle-based method has one big disadvantage, that is, it is too time-consuming. Therefore, a hybrid grid and particle-based method is recently developed. The macroscopic field is computed by a grid-based method, while microscopic or mesoscopic phenomenon on and over a wall surface is computed by a particle-based method. Doing so, I expect that this hybrid method can improve the accuracy of multi-physics simulations in both quality and quantity. In the final paper and my presentation, the numerical procedures of the hybrid grid and particle-based method is introduced, with showing the numerical results on ice accretion and particle deposition phenomena in a jet engine.

Large Deformation Analysis with Connecting Shell and Solid Elements by Using Nitsche's Method

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ABSTRACT

Structures can be constructed with various shape of components which can be modeled as solids, plates, and beams. In the finite element analysis, the whole domain of such structures is often discretized with one type of element only. This approach does not seem to be appropriate in general cases, and it may indicate difficulty in some cases. For example, in the structure composed with an assemblage of solids and plates, if the whole domain is discretized with continuum elements, the local behavior can be evaluated effectively, but huge computational cost may be required. On the other hand, if the entire region is discretized with structural elements, simple bending behavior of thin-walled structures can be predicted efficiently, but they are not sufficient to evaluate local behaviors. Thus, the more effective procedure of discretizing the whole domain of the problem of interest can be constructed by selecting different types of elements according to the shape. This paper presents a numerical procedure to connect shell and solid elements by using the Nitsche's method[1]. The continuity of displacements can be satisfied approximately with the penalty method[2], which is effective for setting the penalty parameter to a sufficiently large value. When the continuity of only displacements on the interface is applied between shell and solid elements, an unreasonable deformation may be observed near the interface. In this work, the continuity of stress vectors on the interface is considered by employing the Nitsche's method, and hence a deformation on the interface can be improved. Several numerical examples of large deformation analysis are presented to examine the fundamental performance of the proposed procedure. The behavior of the proposed simulation model is compared with that of the whole domain discretized with solid elements only. [1] J. Nitsche: Über ein variationsprinzip zur Lösung von Dirichlet-Problemen bei verwendung von teilräumen, die keinen randbedingungen unterworfen sind, *Abhandlungen aus dem Mathematischen Seminar der Universität Hamburg*, 36, 9–15, 1971. [2] G. R. Liu, S. S. Quek: *The Finite Element Method: A Practical Course*, 2nd eds., Butterworth-Heinemann, 2013.

Analysis of Brick Masonry Structures for Coke Oven Using the Hybrid-type Penalty Method

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ABSTRACT

The coke oven which produce coke by carbonization of coal is one of high temperature furnaces in the iron and steel industry and cokes are used to improve efficiency of operation for blast furnace. The walls of coking chamber are brick masonry structures using over 20000 shaped bricks(per chamber) and are subject to repeated thermal and mechanical stresses during operations of the coal charging , carbonization and coke discharging in daily. As the results, chamber walls will be damaged associated with their characteristics in multi-body contact structures and showed complex behavior such as deformation with joint opening, wall thinning, crack initiation and its growth(through crack), corner defect of brick , collapse of wall etc. A numerical predictions of these phenomena are effective not only stable operation and prolonging life of structures but also optimal design of brick structures for damage prevention. To meet above needs, analysis tool of brick masonry structures using the Hybrid-type Penalty Method(HPM)[1] has been developed. In the HPM, analysis field is divided subdomain and the compatibility of the displacement on the element boundary edge is approximately introduced using the penalty as a spring constant of Lagrangian multiplier in the formulation of the hybrid-type virtual work. And surface tractions on boundary of elements are calculated and it is made possible to analyze slip and opening between elements. In this report, outline of development of analysis tool for brick masonry structures using HPM and practical predictions of wall behavior and strength of coking chamber with cracks are introduced. [1] Takeuchi,N. et al.; Development of modified RBSM for rock mechanics using principle of hybrid-type virtual work, pp.395-403 Research Publishing Service, Singapore, 2009

Generation of Three-Dimensional Video Image of Indoor Damage Due to an Earthquake Using Point Cloud

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ABSTRACT

Virtual reality (VR) experience of indoor damage due to earthquake has a great potential for promotion of earthquake-resistant countermeasures and earthquake disaster drill. E-Defense of the National Research Institute for Earth Science and Disaster Resilience, or NIED, possesses the world's largest shaking table by which real scale buildings can be shaken against large earthquake such as the 1995 Kobe earthquake. We aim to develop a VR experience system using data of indoor damage reproduced by E-Defense shake table tests. As data for VR experience system, synchronized video image, sound and floor acceleration were obtained for shake table tests of a 10-story reinforced concrete (RC) structure. Then, VR visualization system was developed in which 360-degree video image which was generated by mapping multiple video images into sphere surface is displayed in a head mount display (HMD) [1]. However, such a 360-degree video image cannot consider the position movement of the user. In this research, we aim to generate three-dimensional video image which can consider the position movement by using point cloud. Shooting target is the same room mentioned above. Firstly, we develop shooting system of point cloud. Kinect v2 is employed to obtain RGB image and depth data. To capture the entire area of the room, eight Kinect v2 devices are installed in this system and network system is constructed to operate synchronized data measurement from outside the shake table. Secondly, to merge data measured at all devices, program that coordinate data of coordinate system of each devices is transformed into those in the unified coordinate system is developed. Finally, to display in a HMD, the amount of data size is eliminated by using voxel grid filter and two different visualization methods are developed; one by using polygon generated by point cloud and another by adjusting the size of the point cloud in accordance with the distance from the view point. In the former case, visualization quality is not satisfactory because data includes negligible noise which leads to zigzag-type elements. In the latter case, VR visualization image to grasp the indoor damage from arbitrary position can be displayed in the HMD. Reference [1] T. Yamashita, M. K. Pal, K. Matsuzaki and H. Tomozawa: Development of a Virtual Reality Experience System for Interior Damage due to an Earthquake -Utilizing E-Defense Shake Table Test-, Journal of Disaster Research, Vol.12, No.5, pp.882-890, 2017.10

A Fully Coupled Finite Element Formulation for Liquid-solid-gas Thermo-fluid Flow with Melting and Solidification and Its Application to Additive Manufacturing

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ABSTRACT

Many important industrial processes, such as additive manufacturing, involve rapid mass, flow and heat transport between gas, liquid and solid phases. Various associated challenges, such as the large density ratio between gas and condensed phases, make accurate, robust thermal multi-phase flow simulations of these processes very difficult. In order to address some of the associated challenges, a computational framework for thermal multi-phase flows is developed based on the finite element method (FEM). A unified model for thermal multi-phase flows similar to the models widely used in the manufacturing community is adopted. The combination of the level-set method and residual-based variational multi-scale formulation (RBVMS) is used to solve the governing equations of thermal multi-phase flows. Phase transitions between solid and liquid phases, i.e., melting and solidification, are considered. Interfacial forces, including surface tension and Marangoni stress, are taken into account and handled by a density-scaled continuum surface force model. A robust fully coupled solution strategy is adopted to handle various numerical difficulties associated with thermal multi-phase flow simulations, and implemented by means of a matrix-free technique using Flexible GMRES. The mathematical formulation and its algorithmic implementation are described in detail. Several numerical examples and the applications to additive manufacturing will be shown. The computational results are compared with analytical, experimental and simulation data from other researchers, with good agreement in cases where such data is available.

Quantifying the Uncertainty of AM Models: from High-fidelity to Low-fidelity

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ABSTRACT

Computational modeling for additive manufacturing has proven to be a powerful tool to understand the physical mechanisms, predict fabrication quality, and guide design and optimization. However, various models have been developed with different assumptions and purposes, and these models are sometimes difficult to choose, especially for end-users, due to the lack of quantitative comparison and standardization. Thus, this study is focused on quantifying the uncertainty due to the modeling assumptions, and evaluating the difference due to whether or not some physical factors are incorporated. Multiple models with different assumptions, from high-fidelity to low-fidelity, are run with a variety of manufacturing process parameters, while experiments are performed to validate the models. The models include: a thermal-fluid flow model resolving individual powder particles, a heat transfer model simplifying powder bed as continuum material and an analytical thermal model. This study will provide guidance on how to select models and how much accuracy to be expected, based on the specific purpose. Moreover, the quantification of each physical factor will also contribute to further developing simplified models, i.e. which factors can be reasonably simplified or ignored. [1] Wentao Yan, Wenjun Ge, Jacob Smith, Stephen Lin, Orion Kafka, Feng Lin, Wing Kam Liu, Multiscale modeling of electron beam melting of functionally graded materials, *Acta Materialia*, 2016. 115: 403-412 [2] Wentao Yan, Wenjun Ge, Ya Qian, Stephen Lin, Gregory Wagner, Feng Lin, Wing Kam Liu, Multi-physics modeling of single/multiple-track defect mechanisms in Electron Beam Selective Melting. *Acta Materialia*, 2017. 134:324-333 [3] Wentao Yan, Ya Qian, Wenjun Ge, Stephen Lin, Gregory Wagner, Feng Lin, Wing Kam Liu, Meso-scale modeling of multiple-layer fabrication process in Selective Electron Beam Melting. *Materials & Design*

Numerical Study on Clad-substrate Interfacial Quality of Laser Cladding for Additive Restoration of Mold Steels Using Crucible Steel

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ABSTRACT

Laser cladding is increasingly used for the repair/restoration of critical structural components in aerospace and automobile industries. To enhance the integrity and functional life of the restored components, improving the clad quality and maintaining the integrity of clad-substrate interface is of primary importance. The quality and life of the restored components will depend on the residual stresses, which are induced due to the temperature gradients, the dissimilarity of the coefficients of thermal expansion and the elastoplastic behavior of the clad and the substrate materials. Further, due to high cooling rates, additional strains are developed due to metallurgical transformation induced plasticity and volumetric dilation. And this temperature gradient and the change in the coefficient of thermal expansion is steep at the interface. Thus the interface can sometimes become the probable cause of weakness of the cladding. In addition, a significant clad diffusion would have occurred across the clad-substrate interface, which affects the microstructure of bonding interface. Complete metallurgical bond between the clad and the substrate is also governed by the melting at the interface. In this study, a coupled metallo-thermomechanical finite element model for laser cladding of CPM9V powder on H13 tool steel is developed to predict the evolution of residual stress due to thermomechanical interactions and metallurgical transformations. This model is employed to predict the transient temperatures, both longitudinal and traverse (to the scanning direction) residual stresses at the clad-substrate interface. To attain minimal dilution, the melt line should lie as close as possible to the clad-substrate interface. This effort of minimize dilution appears to increase the possibility of tensile transverse and longitudinal residual stresses in the clad-substrate interface. Occurrence of a tensile residual stress at the clad-substrate interface could result in the premature failure of the cladding. On the other hand, compressive residual stress at the clad-substrate interface could improve its service life. So the state of the residual stress of the clad-substrate interface is explored. The pre-scanning of the substrate has been noted to improve clad-substrate quality. Micro-hardness is estimated both numerically and experimentally at the clad-substrate interface.

Influence of Various Parameters on the Cutting and Failure Mechanism of Unidirectional CFRP Composites Based on Finite Element Analysis

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ABSTRACT

A three-dimensional micro-scale finite element (FE) model of cutting unidirectional carbon fiber reinforced polymer (UD-CFRP) materials is developed in this paper. Fiber, matrix and the fiber-matrix interface are modeled separately to predict fiber breakage, matrix cracking and fiber-matrix debonding. The fibers are assumed to be linearly elastic up to sudden failure defined by the maximum stress criterion. Matrix material is modeled as elastoplastic in combination with a damage evolution behavior. The debonding at the interface is assumed to occur when the displacements of the cohesive elements exceed their displacement limits. Experiments on orthogonal cutting of UD-CFRP workpiece with various fiber orientations have been conducted and compared to the micro-scale FE predictions. The good correlation between experimental data and numerical results allows for an in-depth FE analysis to explain the cutting mechanism beneath the experimental observations such as cutting forces and surface morphology. The dissipative energies associated with damage in fiber, matrix and the interface, friction in the rake face-composite chip contact zone, friction along the fiber and matrix interface, and plastic deformation of matrix have been evaluated and correlated to the dominating failure mechanisms. The chip formation mechanisms and the surface quality are analyzed and it is found that the former is mainly associated with fiber damage modes, while the latter is related to fiber damage modes and the direction of propagation of fiber-matrix debonding.

Meshless RBF Galerkin Method for Band Structure Calculation of Phononic Crystals

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ABSTRACT

Meshless RBF Galerkin Method for Band Structure Calculation of Phononic Crystals Zhizhong Yan¹, Chuanzeng Zhang² ¹Beijing Institute of Technology zzyan@bit.edu.cn ²University of Siegen In recent years, phononic crystals which are periodically-structured media and possess acoustic/elastic wave band gaps have attracted great attentions due to a variety of important applications. Up to now, some methods have been developed for the calculation of acoustic/elastic wave band gaps, including the plane wave expansion (PWE) method, the wavelet method, the finite element method (FEM) and so on. These methods have their own advantages and disadvantages. Therefore, it has been one of the main contents of phononic crystals research to find the accurate and efficient numerical methods. Recently, meshless methods based on radial basis functions (RBFs) have become attractive for solving partial differential equations (PDEs) using a set of nodes within the domain of interest. In this paper, a new meshless RBF Galerkin (weak form) method is proposed for modeling phononic crystals. When modeling the phononic crystals an eigenvalue problem with periodic boundary conditions is formed. The wave equation is transferred into an integral form by the variational principle, the unknown functions are approximated by a set of RBFs, then the eigenvalue problem of a general matrix is obtained. The Gauss integral method is used to improve the accuracy and solve the discontinuity of the material parameters of phononic crystals. The results obtained from the meshless RBF weak form method are found to be in good agreement with the wavelet method. Meshless RBF local weak form method has obvious advantages compared with the traditional numerical methods. It does not require a grid or mesh, and the RBF is defined as the distance function, which is not sensitive to the dimension. Meanwhile, the use of RBFs for the problems with a discontinuity of material parameters is found to reduce the Gibbs phenomenon. In addition, the Gauss integral method is used to calculate the numerical integral, and the calculation speed is improved as compared to the traditional method. The proposed meshless method are proved to be a promising scheme for calculating the band gaps. References [1] Sigalas M M, Soukoulis C M. Elastic-wave propagation through disordered and/or absorptive layered systems. *Phys Rev B*, 1995, 51: 2780—2789 [2] G.R. Liu, Y.T. Gu, A meshfree method: meshfree weak-strong (mws) from methods, for 2-d solids, *Journal of Computational Mechanics* 33 (1) (2002) 2–14

A MICROMECHANICS-BASED HIERARCHICAL COMPUTATIONAL MODEL TO PREDICT FUNCTIONAL BEHAVIORS OF ELECTRIFIED CEMENTITIOUS COMPOSITES

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Key words: Micromechanics, Hierarchical approach, Cementitious composites, Functional Filler, Genetic algorithm

Abstract. The cementitious composite with functional fillers has attracted with considerable attention in the major scientific and engineering field due to its excellent mechanical and functional characteristics such as high load-carrying capacity and self-detecting of damage. With increasing interest in this multi-functional material, the need for advanced computational modelling such as multiscale modelling has also grown significantly. In this study, a hierarchical computational model based on micromechanics and genetic algorithm is proposed to predict functional behaviors of electrified cementitious composites. In order to consider the tunnelling effect and interface characteristics of conductive fillers in the electrified cementitious composite, the Cauchy's probabilistic model is applied to the concept of an effective medium theory. The model parameters regarding conductive network are estimated by genetic algorithm, and the determined parameters are applied to the micromechanical model. Based on the proposed hierarchical approach, a series of numerical simulations including the experimental comparisons of the electrified cementitious composites with functional fillers are carried out to elucidate the potential of the proposed model.

1 INTRODUCTION

Cementitious material is one of the widely used traditional materials in the civil infrastructure applications owing to its stable mechanical and chemical properties [1]. Recently, the request for multifunctional characteristics is being imposed upon the cementitious material as well as its original functionality such as high load-carrying capacity. As a result, the cementitious material with functional fillers has attracted with considerable attention due to their excellent mechanical and functional characteristics. Among a variety of functional characteristics, the most studied area is conductive cementitious material that can be utilized for electromagnetic shielding [2], self-monitoring [3], deicing pavement [4], etc.

With increasing interest in these multi-functional materials, the need for advanced computational modelling such as multiscale modelling has also grown significantly. In this study, a computational method that quantitatively predicts the functional characteristics of electrified cementitious composite is proposed. A hierarchical computational model based on micromechanics and genetic algorithm is developed, and the electrified cementitious composite corresponding to the mixing ratio of multi-walled carbon nanotube (MWCNT) and carbon fiber (CF), and the water-cement ratio (w/c) is experimentally tested. The experimentally measured data are utilized to estimate the model constants of the proposed method. Figure 1 shows a schematic illustration of MWCNT and CF-embedded cementitious composite considered in this study.

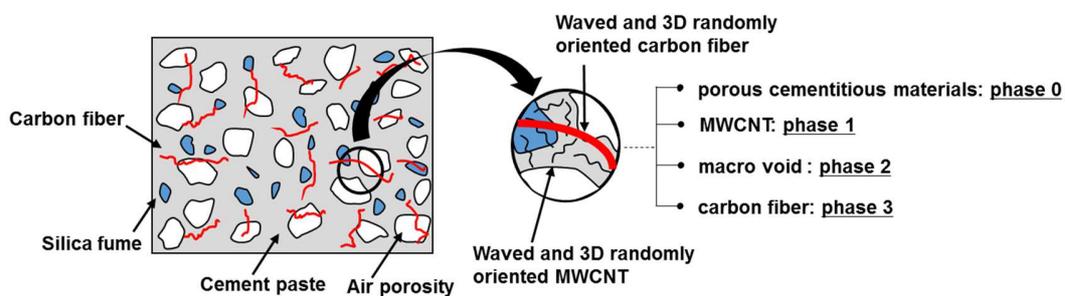


Figure 1. Schematic illustration of MWCNT and CF-embedded cementitious composite

In order to consider the tunneling effect and interface characteristics of conductive fillers in the electrified cementitious composite, the Cauchy's probabilistic model is applied to the concept of an effective medium theory [5]. The model parameters regarding conductive network are estimated by genetic algorithm, and the determined parameters are applied to the micromechanical model [6]. Based on the proposed hierarchical approach, a series of numerical simulations including the experimental comparisons of the electrified cementitious composites with functional fillers are carried out to elucidate the potential of the proposed model.

2 MICROMECHANICS-BASED HIERARCHICAL COMPUTATIONAL MODEL

As shown in Figure 1, this study deals with the electrified cementitious composite having the cementitious material, MWCNT, CF, and porosity. Let us consider the multi-phase material which consists of cementitious material (phase 0), MWCNT (phase 1), porosity (phase 2), and CF (phase 3). It is assumed that the MWCNT, porosity, and CF are randomly and uniformly dispersed in the cementitious material as shown in Figure 1. To simulate the functional behavior of the electrified cementitious composite theoretically, we carried out a micromechanics-based homogenization process consisting of three steps as shown in Figure 2.

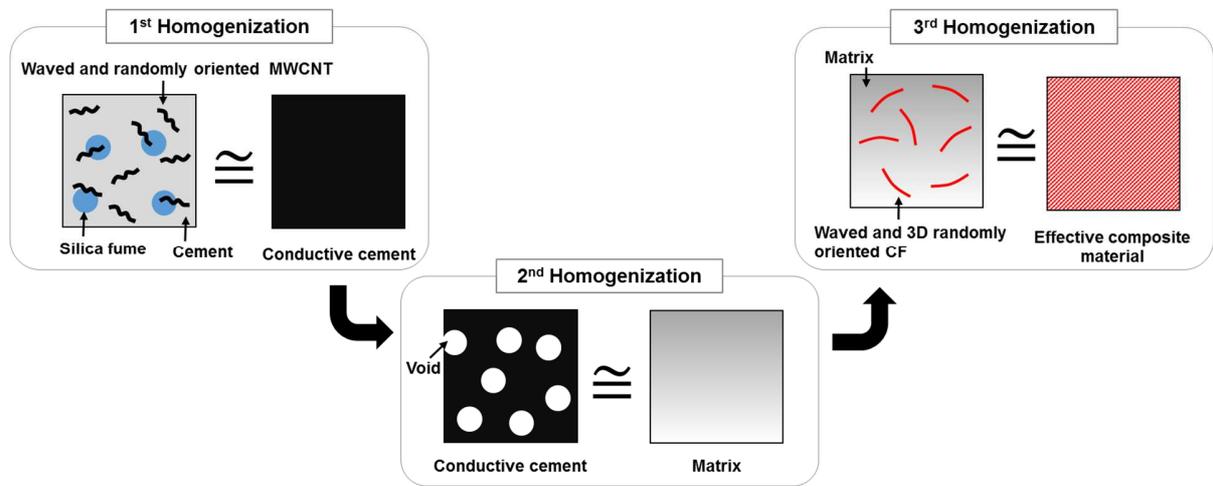


Figure 2. Schematic of micromechanics-based homogenization process consisting of three steps

For homogenization, the effective medium theory (EMT) [5] and the modified Mori-Tanaka (MT) [7] models are considered herein. The EMT and MT models have proven to be suitable theory for predicting the electrical conductivity of composite through many literatures. The effective conductivity of electrified cementitious composites can be expressed as follows using EMT and MT model:

$$(1 - \phi_1) \left[(\mathbf{L}_0 - \mathbf{L}_{cc})^{-1} + \mathbf{L}_0^{-1} / 3 \right]^{-1} + \phi_1 \left[\left\{ (\mathbf{L}_1)^t - \mathbf{L}_{cc} \right\}^{-1} + \mathbf{S}_1 \mathbf{L}_{cc}^{-1} \right]^{-1} = 0 \quad (1)$$

$$\mathbf{L}_m = \mathbf{L}_{cc} + \phi_2 \left[\mathbf{I} - \phi_2 \mathbf{T} : \mathbf{L}_{cc}^{-1} / 3 \right]^{-1} : \mathbf{T} \quad (2)$$

$$\mathbf{T} = \left\{ (\mathbf{L}_2 - \mathbf{L}_{cc})^{-1} + \mathbf{L}_{cc}^{-1} / 3 \right\}^{-1} \quad (3)$$

$$(1 - \phi_3) \left[(\mathbf{L}_m - \mathbf{L}_c)^{-1} + \mathbf{L}_m^{-1} / 3 \right]^{-1} + \phi_3 \left[\left\{ (\mathbf{L}_3)^t - \mathbf{L}_m \right\}^{-1} + \mathbf{S}_3 \mathbf{L}_c^{-1} \right]^{-1} = 0 \quad (4)$$

where \mathbf{L}_r denotes the electrical conductivity of r -phase, and the subscripts cc , m , and e mean the conductive cement, matrix, and effective composite material at each homogenization stage, respectively. The superscript i denotes the interface between the inclusion and matrix. In addition, \mathbf{S}_r and ϕ_r are the aspect ratio-dependent depolarization tensor [7] which can be estimated by genetic algorithm and volume fraction of inclusions, respectively.

3 CHARACTERISTICS OF ELECTRIFIED CEMENTITIOUS COMPOSITE

The electrical resistivity corresponding to the mixing ratio of MWCNT and CF, and the w/c ratios is measured to investigate the electrical characteristics of multifunctional cementitious composite. Figure 3 shows the electrical resistivity of the specimens with respect to weight fraction of MWCNT and CF, and w/c ratios. Here, F0, F1, and F5 mean that CF is contained in the cement matrix for 0, 1, and 5% by weight ratio, respectively.

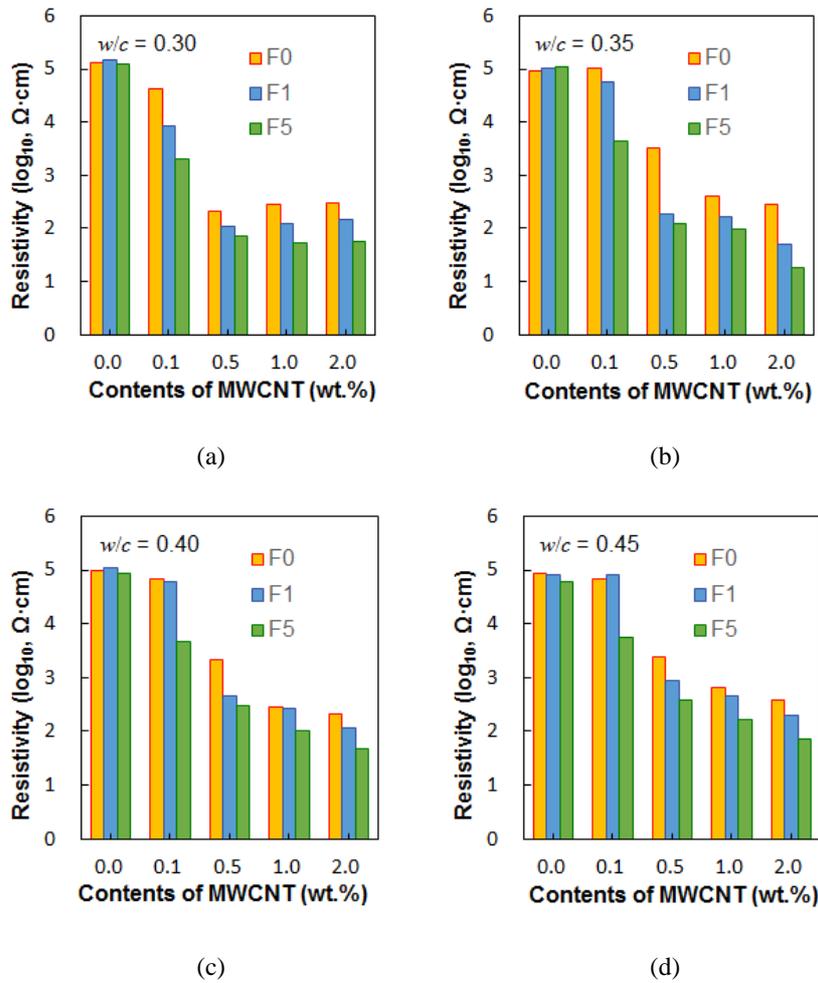


Figure 3. Electrical resistivity of the specimens corresponding to weight fraction of MWCNT, CF, and w/c ratio

Experimental results show that the electrical resistivity of specimens decreases as the amount of MWCNT incorporated into the cement increases, and as the w/c ratio decreases. However, the difference rate of resistivity with the w/c ratio is smaller than that of the reported results from the existing literatures, which is caused by the hierarchical conductive pathway, bridging CF and MWCNT. A related scanning electron microscope (SEM) image that can explain this mechanism (tunneling effect) is shown in Figure 4.

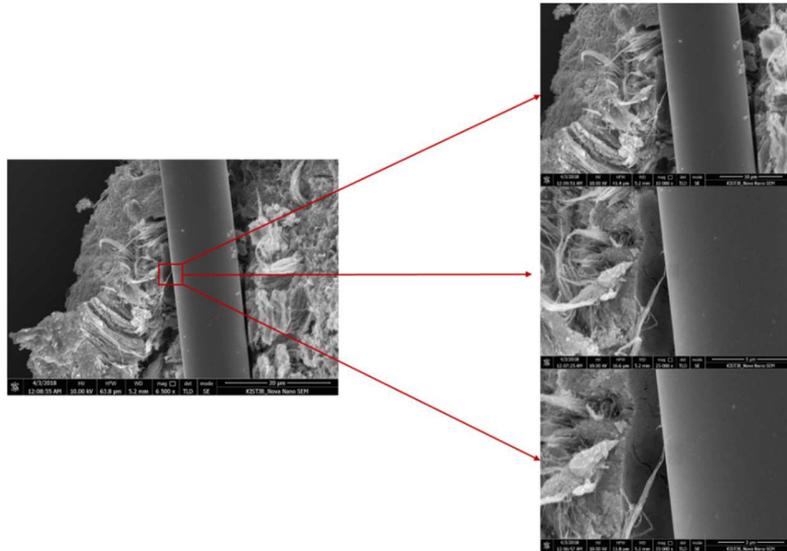


Figure 4. SEM image illustrating hierarchical conductive pathway, bridging CF and MWCNT

4 CONCLUSIONS

This study presents the micromechanics-based hierarchical computational model for electrified cementitious composites. In particular, the proposed computational approach, in which the computational method (micromechanics and generic algorithm) and a series of experiments are properly associated, enables accurate prediction of functional behavior of electrified cementitious composites, not only with respect to electrical properties but also internal conductivity network mechanism. Figure 5 shows the representative comparison of electrical resistivity between predictions and experimental results of electrified cementitious composites, in which the predictions are in good agreement with the experimental results. Although this study is focused on the electrified cementitious composite having MWCNT and CF, the proposed computational approach could be utilized to predict the functional characteristics of the cementitious composites with different functional fillers.

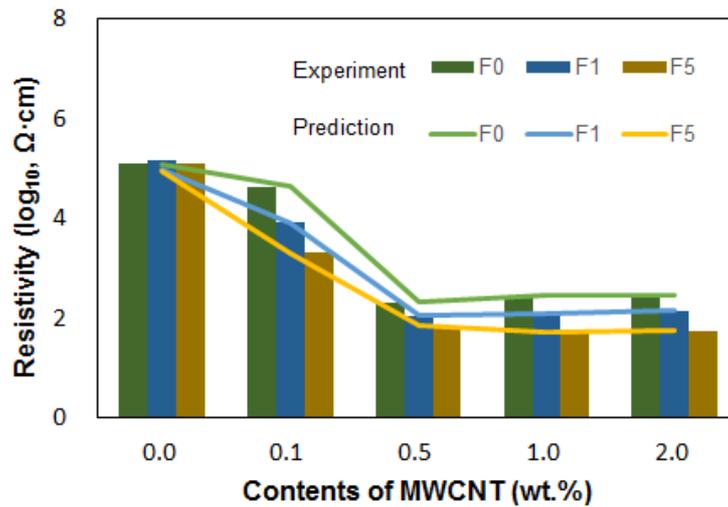


Figure 5. Representative comparison of electrical resistivity between predictions and experimental results of the cementitious composite

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Nonlinear Finite Element Methods and Applications in Automobile Industry

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ABSTRACT

With the rapidly developing computing power, nonlinear finite element methods (FEM) have been widely applied to solve challenging engineering problems. Great research efforts have been devoted to improve the accuracy of the solution and the stability and robustness of the solution process. Some cutting edge research work has been done and become available in commercial finite element software. This paper presents some recent developments in the application of nonlinear FEM, particularly in automobile industry. A few practical industrial cases are presented to show the performance of these developments.

Symplectic Semi-analytical Method for the Multilayered Two-dimensional Decagonal Quasicrystal Plates with Heat Effect

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ABSTRACT

The mixed finite element--symplectic semi-analytical approach is proposed in this article to analyze the multilayered two-dimensional decagonal quasicrystal plates under simply supported displacement boundary conditions with the heat effect. The basic equations of the Hamiltonian formalism is derived by introducing the total free energy functions composed by the phonon field and the phason field. The problem is solved in an in-plane finite element discretization in a single layer and then in the multilayer solution with the symplectic state space method. The correctness of the proposed semi-analytical method is verified with open literature. Numerical results show that stacking sequences, coupling constants and thermal fields take a great role in the stress fields of the multilayered quasicrystal plates. The numerical results can also be used as analyzing laminated composites made of two-dimensional quasicrystals.

NONLINEAR ANALYSIS OF UNDERWATER MARINE RISER RECOIL USING HIGHLY EFFICIENT MULTIBODY DYNAMICS METHOD

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Key words: Marine Riser; Flexible Multibody Dynamics; Recoil; Auxiliary Pipelines; Nonlinear Analysis.

Abstract. A flexible multibody methodology for full-scale marine riser system considering static, modal and recoil case is presented in this paper. Lagrangian equations together with numerical methods for static, modal and emergency disconnect recoil cases are developed in detail. Finite element method has been widely used in the recoil research of marine riser in the recent decades, but the corresponding applications of multibody dynamics still consider the riser with finite segment method or directly simplify it as a mass-spring system to make the number of degrees of freedom of system small. In this paper, a full-scale flexible multibody dynamics model of marine riser is built with geometrically exact beam that is modified for ocean environment in 1547-meter water depth and mud discharging. A numerical example is built and calculated for static, modal and recoil cases to compared with the commercial finite element software DEEPRISER, 93% agreement is gained for all cases and the presented flexible multibody method is 3 time faster in the recoil case. The auxiliary pipelines on the riser are always simplified by an equivalent mass which is added to that of marine riser in the finite element method. To verify this, a more detailed example is built with the auxiliary pipelines modeled by respective beam lines and connected to riser by hundreds of constraint joints. The associate mass model of auxiliary pipelines is only suitable for static and modal calculation, but not for the recoil dynamic calculation, where the dangerous case of riser may be mistakenly seen as safe case. But the simplified model considering both associate mass and associate stiffness is suitable for recoil dynamic calculation which is almost the same as the detailed auxiliary model.

1. INTRODUCTION

The methods of studying marine riser system can be mainly divided into three categories: analytical method ^[1-6], finite element method ^[7-19] and multibody dynamic method ^[20-21], along with real tests on drillships ^[12,29-31] and increasing interests in nonlinearity of riser recoil ^[11-19,29-31] and drillstring/riser involved contacts ^[22-24,27-28].

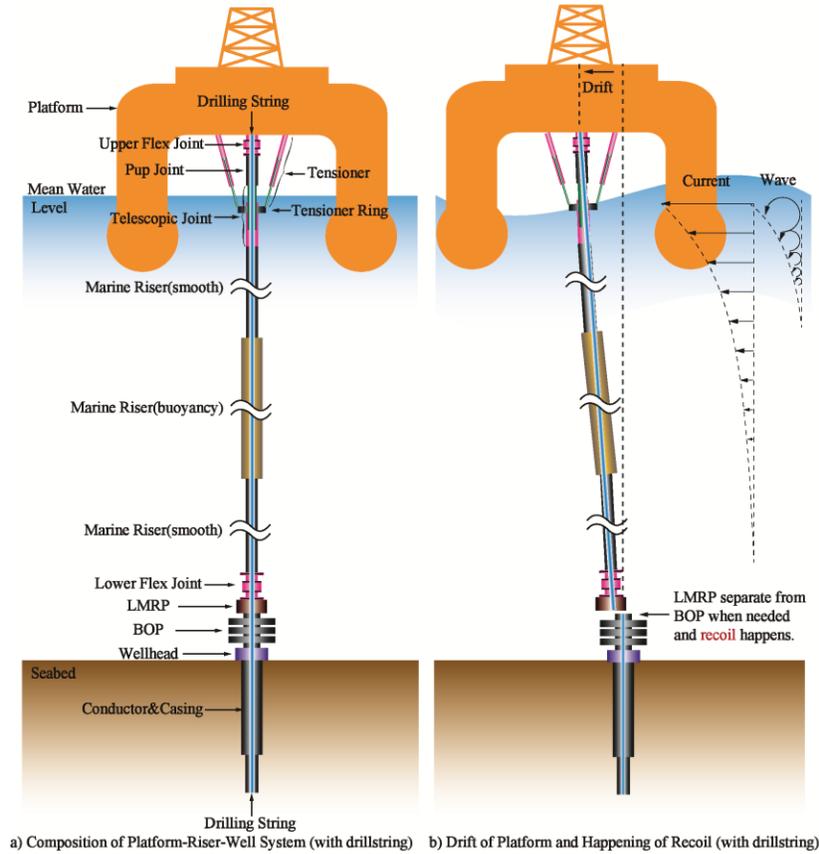


Fig. 1 Platform-Riser-Well System

Analytical equations of marine riser mechanics are built in differential equation form and intuitive conclusion can be derived with some basic simplification. Then either with series solution method ^[1] employed by Fischer and Ludwig, or with finite difference methods used by Tidwell, Ilfrey ^[2] and Sexton ^[3], or with Runge Kutta integration method applied by Burke ^[4], these equations are solved. Systematic analysis methodology for various issues of marine riser has been summarized in specific books ^[5-6], where ^[5] uses excel files to verify the findings by comparing with the results of different calculation methods and ^[6] focuses on closed form solutions of static and dynamic stable solution mainly by series solution method.

Finite element method has been the major tool for marine riser analysis in the recent decades. In 1973, Gardner and Kotch ^[7] took the small angle, large deflection theory in the finite formulation of riser, then Gnone ^[8] considered the three-dimensional case in 1975, followed by Kirk ^[9] who employed normal mode solution for dynamic response in 1979, and Bernitsas ^[10] presented a large deformation within small strain theory and coupled the torsion and bending in

1985. With the development of nonlinear theory, a number of specific commercial software based on finite element method have developed their methodology respectively on simulating the disconnect and recoil of marine riser. Yong and Hock^[11-13] compared the 3700-ft-water-depth emergency disconnect analysis results of a modified RISTEN program with that of a full-scale test on drillship Discover 534 in 1992; Lang and Real^[14] employed iterative procedures to solve differential equations for tensioner and finite volume equations for mud column respectively in the recoil analysis with software DEEPRISER, and several static and dynamic stages were proposed to get the initial status of the detailed tensioner; Grytøy and Sharma^[15-16] proposed a disconnection analysis methodology for simulating the CWO riser and drilling riser in software RIFLEX, and more detailed description can be found in the theses of Brynstad^[17] and Grønevik^[18]. Pestana^[19] also introduced a method of recoil simulation in software ORCAFLEX. The marine riser system researches based on finite element software take the advantages of built-in ocean environment loads and riser flexibility, but suffer from simulating moving joints and numerical stiffness caused by realistic tensioner spring coefficients and recoil impulse.

There are only a few applications of multibody dynamics in the marine riser system. In 2003, Raman^[20] used the Kane's formalism to build the marine riser with lumped masses which were connected by extensional and rotational springs, and Runge-Kutta method is chosen to integrate in MATLAB, 3.86 hours were spent for a 500s simulation with 10 lumped masses on a Pentium III PC. In 2015, Lee^[21] employed the discrete Euler-Lagrange equation of rigid multibody dynamics for wireline tensioner simulation with realistic tension spring coefficient, where the tensioner was modeled with 6 rigid bodies and the riser simplified as a mass-spring-damping system. Full-scale model with flexible riser and corresponding efficient numerical scheme for large degrees of freedom haven't been developed for the steady/recoil research of marine riser system.

A methodology for full-scale flexible riser system based on multibody dynamics is presented in this paper, Lagrangian equations together with numerical methods for static, modal and emergency disconnect recoil cases are developed in detail, in which a highly efficient algorithm for drillstring-riser contact is proposed. In the first section, the modeling of marine riser system in flexible multibody dynamics is presented. In the second section, example based on realistic drillship is performed and the numerical results of static, modal and recoil cases are compared with those of finite element commercial software DEEPRISER to verify the correctness and efficiency of the proposed method. In the third section, a detailed auxiliary pipelines model is analyzed and corresponding simplification rule for FEM method is suggested.

2. MODELING OF MARINE RISER SYSTEM IN FLEXIBLE MULTIBODY DYNAMICS

In the flexible multibody model, the pup joints, telescopic joint, marine riser, drillstring and conductor in the soil are discretized with beam elements; other parts are simplified as rigid bodies. The marine beam element for marine riser and drillstring is based on the ordinary beam element, with considering hydrostatic, hydrodynamic and friction loads on the inner and outer surfaces of the riser.

The upper flex joint (UFJ) is simulated by a ball hinge together with a group of torsion springs, and it is the same to the lower flex joint (LFJ). Two cylindrical pairs are set respectively at the upper end of the telescopic cylinder and the lower end of the telescopic rod. A ball hinge connects the tensioner rod and the tensioner ring at an offset from the center line of the

telescopic joint. The lower end of the conductor is constrained to the seabed with a ball hinge. The drillstring is connected to platform with a ball hinge + torsion springs, although there is another tensioner subsystem for drillstring, a simplicity of ball hinge connection is enough for the simulation of contact between drillstring and riser.

The marine riser disconnect is simulated by releasing the time-dependent fixed hinge between LMRP and BOP at a given time, to make the recoil analysis. This model is also applicable for a system with wire line tensioner, with a slight adjustment by removing the tensioner rod and replacing direct-acting tensioner force with wire line tensioner force.

2.1 Lagrange governing equation

Lagrange equations of the first kind is adopted to state the flexible multibody system [29] in this paper, it costs additional number of degrees of freedom for constraint multipliers to avoid degrees merging of linked bodies introduced by the second kind, but it is fortunate that the additional degrees of freedom of constraint multipliers is quiet small compared to those of flexible parts with finite element discrete format (not simplified flexible body with modal method). The system governing equations are

$$\begin{cases} \underbrace{\frac{d}{dt} \left(\frac{\partial L(\mathbf{q}, \dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}} \right) - \frac{\partial L(\mathbf{q}, \dot{\mathbf{q}})}{\partial \mathbf{q}} + \mathbf{F}_{ex}}_{\mathbf{F}_L} + \left(\frac{\partial \Phi}{\partial \mathbf{q}} \right)^T \boldsymbol{\lambda} = \mathbf{0} \\ \Phi(\mathbf{q}) = \mathbf{0} \end{cases} \quad (1)$$

wherein t is the time variable, $\mathbf{q} \in \mathbb{R}^{n_q}$ is the general coordinate of rigid and flexible bodies, $\boldsymbol{\lambda} \in \mathbb{R}^{n_\lambda}$ is the Lagrange multiplier of constraints, $L(\mathbf{q}, \dot{\mathbf{q}}) = T - V$ is the Lagrange function with kinematic energy T and potential energy V , $\Phi(\mathbf{q})$ is the equations for complete constraints of number of degrees n_λ . The potential general force gained from Lagrange function is also noted as \mathbf{F}_L , together with general force of non-potential force $\mathbf{F}_{ex}(\mathbf{q}, \dot{\mathbf{q}}, t)$ and constraint force $\left(\frac{\partial \Phi}{\partial \mathbf{q}} \right)^T \boldsymbol{\lambda}$ to get a zero vector.

The following work to assemble the governing equations of the platform-riser-well system is to give out the detailed expression of \mathbf{F}_L and \mathbf{F}_{ex} for rigid body and marine riser, and constraints Φ between them. Ocean environment loads such as sea current, sea wave, internal load i.e. mud discharge friction force are considered.

2.2 Geometrically exact beam

Geometrically exact beam^[30-31] with rotation vector as attitude parameter is adopted to present the quality and elasticity of marine riser. A total Lagrangian framework is chosen for beam as the marine riser for drilling is normally stiff enough to stay in the linear elastic constitutive model.

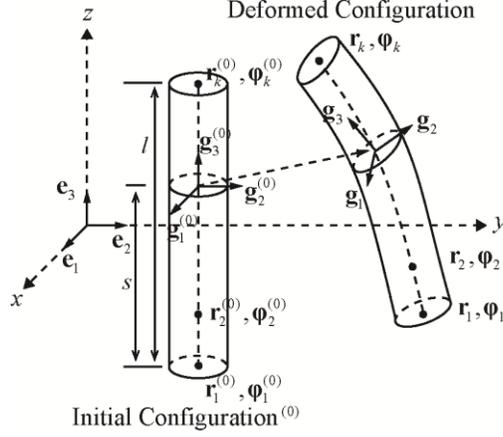


Fig. 2 Initial and Deformed Configuration of Beam

As shown in Fig. 2, if there is k ($2 \sim 5$) nodes in an element, each node takes 6 coordinate $(\mathbf{r}_i, \varphi_i)$ as general coordinate just as that of a rigid body. The shape functions note as $N_i(\xi)$, where $\xi = s/l$ is the normalized length along the beam axis, s is the arc length, l is the element length. Then the position and attitude at ξ is interpolated with

$$\begin{aligned} \mathbf{r}(\xi) &= \sum_{i=1}^k N_i(\xi) \mathbf{r}_i \\ \boldsymbol{\varphi}(\xi) &= \sum_{i=1}^k N_i(\xi) \boldsymbol{\varphi}_i \end{aligned} \quad (2)$$

2.3 Current & wave & mud discharging

Morison empirical formula is adopted to simulate the force of wave and current ^[15-16]

$$F_{morison} = \rho \pi \frac{D^2}{4} C_m a + \frac{\rho}{2} C_d D |u| u \quad (3)$$

Wherein u is the quantity of relative velocity \mathbf{u} , ρ is the density of sea water, D is the outer diameter of riser, C_m is the coefficient of added mass, C_d is the coefficient of drag, u is the transverse component of relative speed of the sea water to marine riser. The speed vector of sea wave can be calculated with stokes formula or any other wave model.

One-dimensional fluid Euler equation [17] and finite volume method is adopted to form the friction force of discharging mud [18]. After the linear density of friction F_{fric} is calculated, the general force of mud friction is

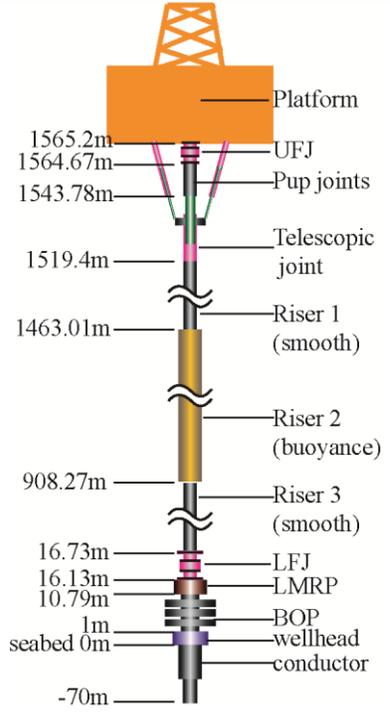
$$\mathbf{F}_{in}^{fric} = \int_0^l F_{fric} [(\dot{\mathbf{x}} \cdot \mathbf{G}_3) \mathbf{G}_3]^T \frac{\partial \mathbf{x}}{\partial \mathbf{q}} dl \quad (4)$$

In addition, hydrostatic pressure should be applied at the section where the interfaces of riser joints have different inside or outside diameter; hydrostatic pressure should be applied to the bottom of LMRP when the rise is cut off under the LMRP to disconnected from the wellhead and the pressured area should the sum of last riser joint's section and those of auxiliary pipelines.

3. NUMERICAL RESULTS

A platform-riser-well model base on a real system is built in both DEEPRISER (a specialized commercial software for marine riser related problems) and homemade codes with the same physical parameters which are shown in Tab. 1 .

Tab. 1 Parameters of Platform-Riser-Well System

		<i>Name</i>		<i>Value</i>			
				Riser/Conductor material	steel		
		Riser element length	3m				
Riser 1	Outside diameter	533.4mm					
	Inside diameter	508.0mm					
	Length of a joint	22.86m					
	Weight in air (a joint)	15331kg					
	Weight in water(a joint)	13335kg					
Riser 2	Outside diameter of buoyance	1371.6mm					
	Outside diameter	533.4mm					
	Inside diameter	511.2mm					
	Length of a joint	22.86m					
	Weight in air(a joint)	14605kg					
	Weight in water(a joint)	12700kg					
Riser 3	Buoyance weight in air(a joint)	9661 kg					
	Buoyance Weight in water(a joint)	-11022 kg					
	Outside diameter	533.4mm					
	Inside diameter	514.4mm					
	Length of a joint	22.86m					
LMRP	Weight in air (a joint)	13698kg					
	Weight in water(a joint)	11929kg					
	Weight in air	148846kg					
Auxiliary pipeline	Weight in water	129496kg					
	<i>Serial number</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>	<i>6</i>
	OD(mm)	152.4	152.4	127	63.5	63.5	66.7
ID(mm)	101.6	101.6	101.6	50.8	50.8	50.8	

3.1 Equilibrium, Vibration and Recoil Results

The comparison of equilibrium configuration results is shown in Fig. 3, horizontal displacement of riser under different drift off values of platform are compared.

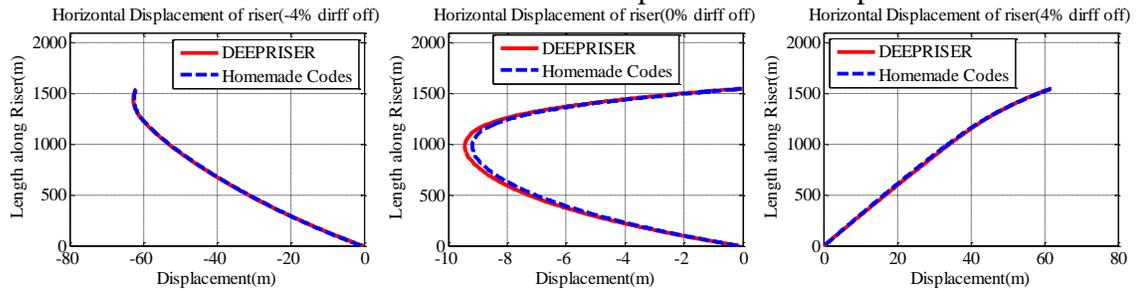


Fig. 3 Equilibrium Results of -4%,0%,4% Drift Off (current, top tension 5800kN)

The comparison of vibration results around equilibrium configuration is shown in Fig. 4, the vibration is calculated under 0% drift off of platform with once a year current. Natural frequency and vibration mode near the equilibrium configuration are compared. The top tension is set as 5800kN.

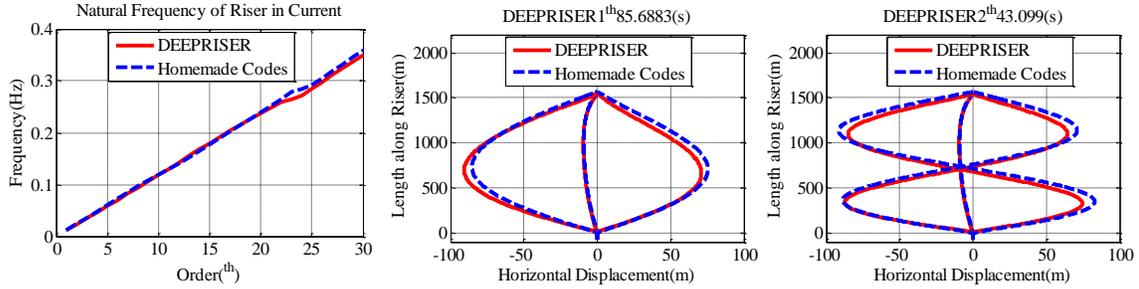


Fig. 4 Vibration Results Under 0% Drift Off (current, top tension 5800kN)

The comparison of recoil results is shown in Fig. 5, the LMRP is cut off at 46th second, numerical results of 4 mainly engineering criteria are compared, including telescopic joint stroke, tensioner ring tension, elevation of LMRP, and envelope of effective tension of riser.

As shown in Tab. 2, a minimum coincidence degree of 93.4% is gained between DEEPRISER and the homemade codes with presented flexible multibody dynamic method. The results of DEEPRISER are set as reference values for the calculation of coincidence degrees, and the coincidence of recoil is the minimum of coincidence degrees of the four criteria.

Consider the method difference between DEEPRISER and homemade codes, the results of homemade codes are verified to be correct for equilibrium configuration calculation, vibration calculation and dynamic response of recoil calculation.

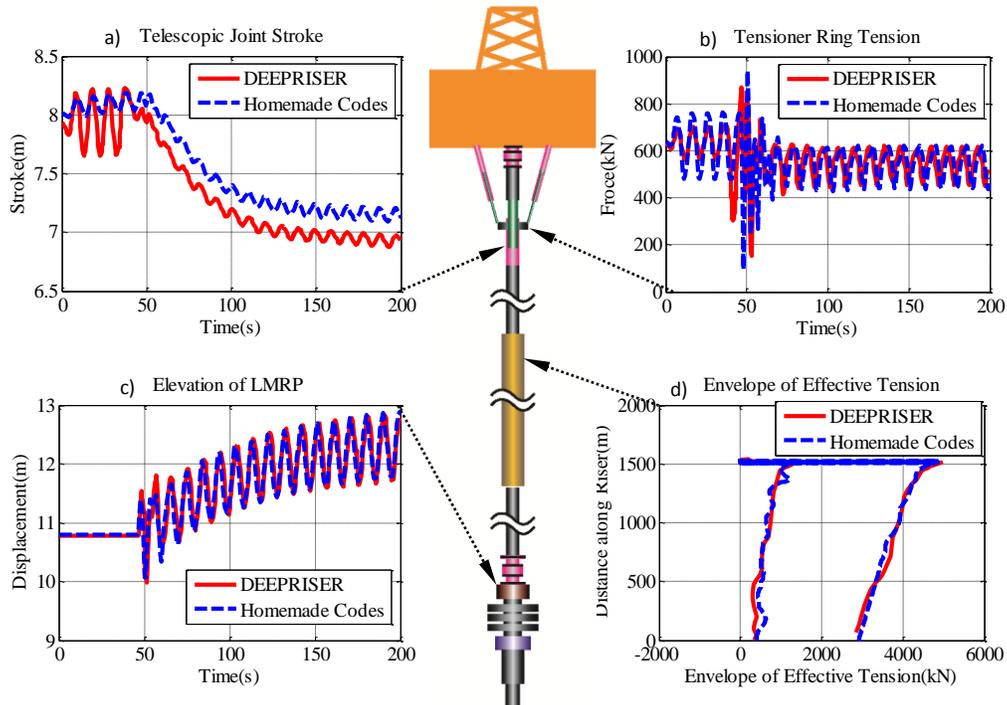


Fig. 5 Recoil results of dynamic response (wave, current, 0% drift off, top tension 3500kN)

Tab. 2 Coincidence between DEEPRISER and The Homemade Codes

<i>Case</i>	<i>Equilibrium</i>			<i>Vibration</i>	<i>Recoil</i>
Items	-4% drift off	4% drift off	0% drift off	frequency	
Coincidence	98.2%	95.8%	93.4%	95.1%	93.5%

3.2 Efficiency of flexible multibody method

The recoil model is calculated by DEEPRISER and the homemade codes on the same computer with configuration, although parallel computing is available for the homemade codes, single core mode is set for the homemade codes to keep the same with DEEPRISER in the efficiency comparison of recoil simulation. As shown in Tab. 3, the homemade codes gained a X3.2 speed up compared to DEEPRISER, mainly because the step sizes in multibody dynamics are much bigger than those of DEEPRISER as shown in Fig. 6. The multibody dynamics adopts smart variable step-size implicit integration algorithm of BDF, however DEEPRISER uses constant-step-size explicit algorithm in recoil simulation so far.

Tab. 3 CPU Time for Recoil Calculation (single core)

<i>Software</i>	<i>CPU time</i>
DEEPRISER	12min
Homemade Codes	3.7 min
Speed up	3.2

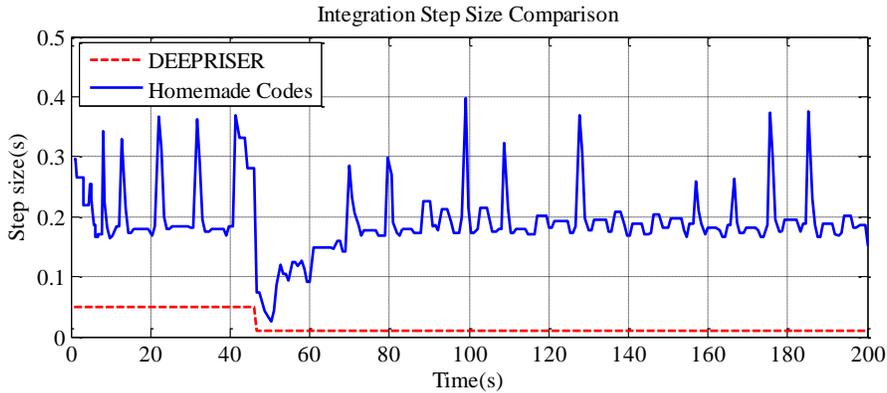


Fig. 6 Integration Step Size Comparison

4. Detailed auxiliary pipeline model

In the modeling of the marine riser in many FEM commercial software simulating marine riser system, including DEEPRISER, the auxiliary pipelines are considered by added mass which is uniformly applied to the riser and the stiffness of auxiliary pipelines is ignored. As shown in Fig. 7 a), only the mass contribution of auxiliary pipelines is considered. However, in flexible multibody dynamics, it is very easy to connect flexible parts, rigid parts with constraints and the method can allow many constraints in the system and encounter no problem in numerical

calculation. So as shown in Fig. 7 b), a detailed auxiliary pipeline model is considered and calculated with flexible multibody dynamics. Each pipeline is simulated with a beam and they are connected to the riser at every joint end by fixed constraints. For 6 auxiliary pipelines in the model, there are more than 300 fixed constraints in the detailed auxiliary model and the number of degrees of freedom is multiplied by more than 7 times. To make a complete comparison, a model considering both added mass and added stiffness of auxiliary pipelines is also built and calculated.

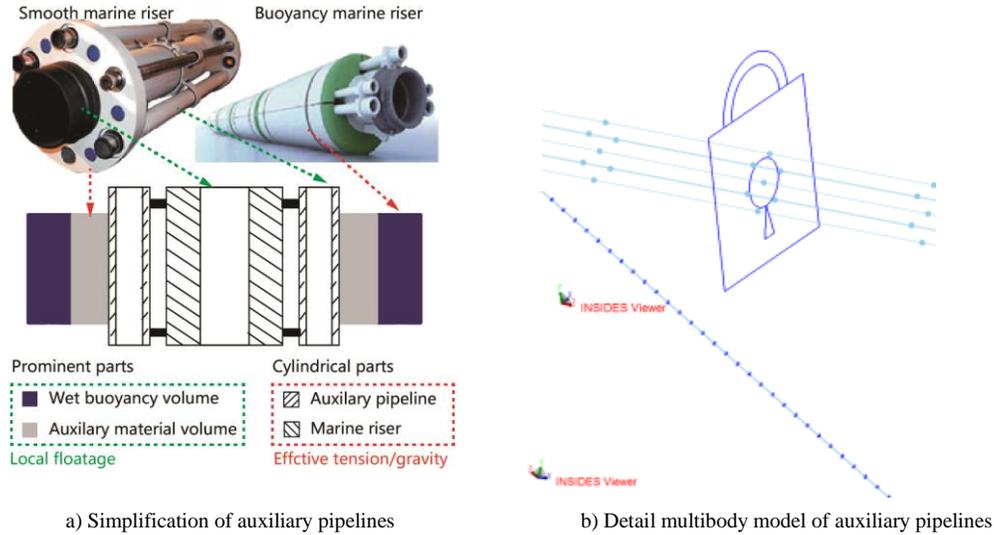


Fig. 7 Detailed Flexible Multibody Model

The calculated results are shown in Fig. 8~Fig. 9 for static equilibrium, vibration modes and recoil dynamics. The results are summarized in Tab. 4, it shows for static calculation, the added mass model of auxiliary pipelines is only suitable for static and modal calculation, but not for the recoil dynamic calculation, where the dangerous case of riser may be mistakenly seen as safe case. But the simplified model considering both added mass and added stiffness is suitable for recoil dynamic calculation which is almost the same as the detailed auxiliary model.

Tab. 4 Results Summary of Detailed Auxiliary Model

<i>Analysis Type</i>	<i>Detailed Model</i>	<i>Multibody</i>	<i>Single Beam (Associate Mass)</i>	<i>Single Beam (Associate Mass & Stiffness)</i>
Static	Ref.		✓	✓
Modal	Ref.		✓	✗
Recoil	Ref.		✗	✓

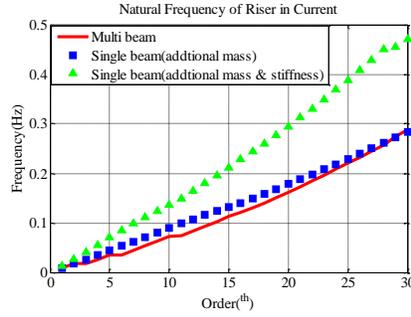


Fig. 8 Vibration Results Under 0% Drift Off (current, top tension 5800kN)

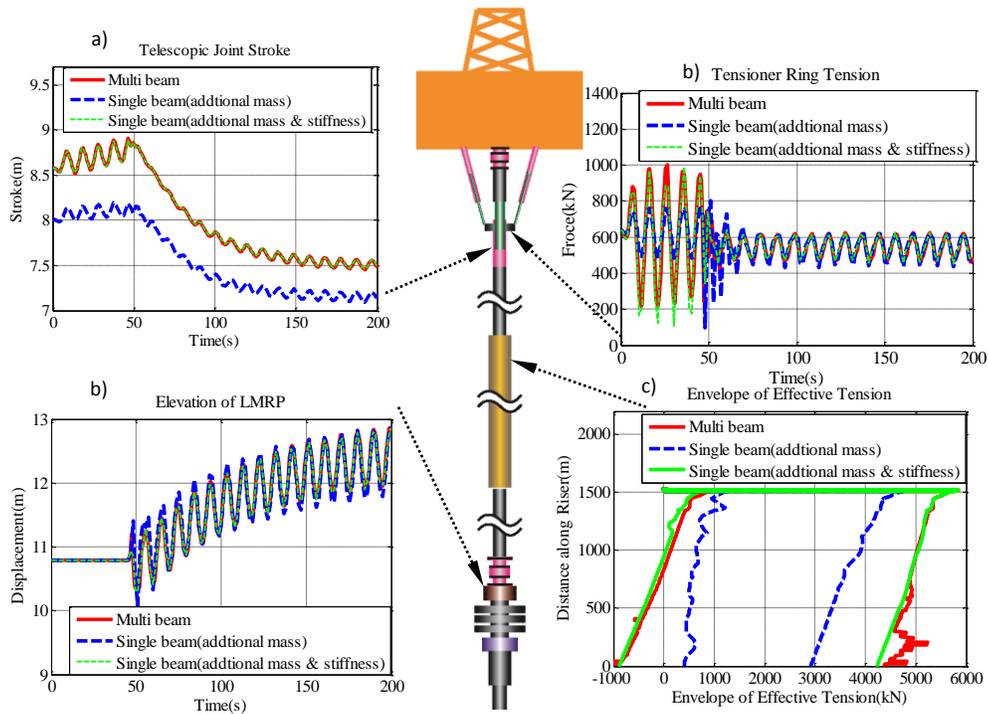


Fig. 9 Recoil Results of Dynamic Response (wave, current, 0% drift off, top tension 3500kN)

5. CONCLUSIONS

This article models the marine riser system in flexible multibody dynamics considering static, modal and recoil cases in full-scale. Lagrangian equations of first class and geometrically exact beam are adopted to present the riser system. Buoyance, wave, current and mud discharge are included in the numerical calculations. Basic examples coincide with DEEPRISER, a commercial marine riser software with FEM method, and gains 3 times speedup. Detailed auxiliary pipelines model is built in flexible multibody dynamics and the results show that the simplified model considering auxiliary pipelines as associate mass may lead to wrong estimation of safety in the recoil simulation. It suggests the associated stiffness should also be included if simplify the auxiliary pipeline in recoil case, but the static and modal cases could ignored it.

ACKNOWLEDGEMENT

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The Multi-scale Modeling for Progressive Failure Analysis of Woven Composite Using Domain Superposition Technique

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ABSTRACT

A robust multi-scale computational strategy allowing reliable prediction of the progressive failure behaviors is developed for woven composite, which can deal with the mesh generation for arbitrary architecture. In micro-scale modeling, the statistical representative volume element (SRVE) under periodic boundary condition (PBC) is setup to approximate the microstructure of the composite using initially periodic shaking method. For the matrix, the elastic-plastic model taking into account hydrostatic stresses is introduced, as well as ductile damage criteria. Cohesive zone model based on the power law is used to simulate the fiber/matrix debonding whose parameters are explored in details. In the meso-scale approach, the Hashin criteria is formed for yarn to predict the damage initiation in progressive damage model, with Von Mises criteria being considered for matrix since the main failure mechanism is dominated by the fracture in yarns [1]. In order to overcome the difficulty in mesh partition due to the complex internal architecture and geometric degeneracies, the domain superposition technique (DST) is proposed to realize fast modeling in FEA. The model adopts the global domain geometry superimposed with the reinforcement phase material domain geometries, therefore, facilitating the generation of hexahedral elements, which is also easy to apply PBC. Using the DST model, the reinforcement FE meshes are couple into global mesh by nodal degree of freedom coupling technique. Accordingly, the material models of reinforcement phase are adjusted to ensure the accurate representation of the actual composites system. The above multi-scale progressive damage model is incorporated into a finite element code ABAQUS, via a user-defined material subroutine. The comparison between the numerical results and experimental data taken from Naik [2] are carried out in terms of stress-strain curves and failure strength. The predictions are in good agreement with the experimental results. The damage process indicates that the warp longitudinal failure occurs first, followed by the fill transverse failure. All these failure modes are accompanied by the failure of matrix until the final fracture caused by the longitudinal failure. The multi-scale modeling approach opens a path to provide accurate prediction in fast parametric modeling. [1] Yuan Zhou et al, Progressive damage analysis and strength prediction of 2D plain weave composites, 47(2013) 220-229 [2] N. K. Naik, V. K. Ganesh. Failure behavior of plain weave fabric laminates under on-axis uniaxial tensile loading:II—analytical predictions, 30 (1992) 1779-1822

Strain Analysis Damage Identification Method for Crane Girder Based on Peridynamics

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ABSTRACT

Peridynamics is a new numerical calculation theory of mechanics, and is widely used in studies of discontinuous mechanical problems, damage simulation and identification and other complex mechanical behaviors. Because of working impact loads, the crane girder is often damaged in the forms of crack initiation and growth. Considering of the advantages of peridynamics, a numerical calculation of strain signals based on peridynamics of the crane girder being subject to working impact loads was studied. In this study, the mathematical model of the crane girder was established, and the strain signals of checkpoints were simulated. By analysis these strain signals, the characteristics of the strain signals was got, the damage mechanism of the crane girder was researched. Firstly, the mathematical model of the crane girder was established based on peridynamics and the working impact load was simulated as weigh emergency braking. Secondly, some checkpoints were arranged in different locations on the crane girder according to sensor optimization theory, and the strain signals of these checkpoints were acquired. Then, the characteristics of the strain signals were obtained through time-frequency analysis, and the relationship of between strain signal and damage degree was interpreted, then the damage mechanism of the crane girder was got. Finally, the application of this method was implemented by some experiments, and the results demonstrated that this method can effectively identify the damage of the crane girder.

A Taylor-based Meshless Method for Non-linear PDEs

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ABSTRACT

In this talk, Taylor series are applied to the spatial discretization of partial differential equations, a topic on which there are very few papers in the literature. As in Trefftz methods, one uses a complete family of quasi-exact solutions of the PDE in each subdomain, which permits to discretize only the boundary and the interfaces. Here the most original point is the algorithm to build these quasi-exact polynomial solutions, by vanishing the Taylor series of the residual. The latter procedure can be applied to generic partial differential systems, possibly by means of algorithmic differentiation, which has been achieved for non-linear Poisson equations (Yang et al, J. Comp. Physics 2017), hyperelasticity or Navier-Stokes equation, including when fluid flows are coupled with double diffusion or heat propagation. Within Trefftz methods, various techniques are available to connect several analytical solutions in various subdomains. Here a meshless integrationless procedure based on least-square collocation is used. This full procedure, called Taylor meshless method (TMM), proves to be robust and efficient. It converges with the degree of the polynomials (p-convergence) and/or with the number of subdomains (h-convergence). As often with Trefftz methods, the main difficulty is the loss of accuracy due to matrix ill-conditioning, but according to a number of numerical tests, the method was able to provide highly accurate solutions (up to 10^{-10}), with a rather large degree (up to $p=15-20$), with a strong reduction of the number of unknowns as compared with classical methods (typically a ratio of 20-50 with respect to FEM) and for large scale problems (the equivalent FEM mesh involving millions of unknowns), see Yang et al, Int. J. Num. Eng. 2017. This talk will focus on applications in fluid mechanics.

Two-Mass Vehicle Model for Extracting Bridge Frequencies

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ABSTRACT

In the past decade, the dynamic response of a passing vehicle has been utilized to extract the frequencies of the supporting bridge. Particularly, the test vehicle was modeled as a single-degree-of-freedom sprung mass moving over a simple beam in most previous studies, which suffers from the drawback that the sprung mass may be affected by the vehicle motion. As such, the present work presents a two-mass vehicle model for extracting the bridge frequencies, which contains a sprung mass (vehicle body) and an unsprung mass (axle mass). By using the response of the unsprung mass, the bridge response can be extracted more realistically. The main results of the present work are listed as follows: (1) with the aid of unsprung mass in the vehicle model, the dynamic responses of both the vehicle and bridge can be faithfully revealed, (2) increasing the unsprung mass can effectively help the extraction of bridge frequencies, including the second frequency, (3) the proposed model can identify the bridge frequencies even under high levels of road roughness, while the traditional single-mass model cannot, and (4) the proposed model can identify the bridge frequencies under high levels of road roughness without additional techniques of processing in the presence of vehicle damping.

Edge Orientations of Mechanically Exfoliated Anisotropic Two-dimensional Materials

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ABSTRACT

Mechanical exfoliation is an approach widely applied to prepare high-quality two-dimensional (2D) materials for investigating their intrinsic physical properties. During mechanical exfoliation, in-plane cleavage results in new edges whose orientations play an important role in determining the properties of the as-exfoliated 2D materials especially those with high anisotropy. Here, we systematically investigate the factors affecting the edge orientation of 2D materials obtained by mechanical exfoliation. Our theoretical study manifests that the fractured direction during mechanical exfoliation is determined synergistically by the tearing direction and material anisotropy of fracture energy. For a specific 2D material, our theory enables us to predict the possible edge orientations of the exfoliated flakes as well as their occurring probabilities. The theoretical prediction is experimentally verified by examining the inter-edge angles of the exfoliated flakes of four typical 2D materials including graphene, MoS₂, PtS₂, and black phosphorus. This work not only sheds light on the mechanics of exfoliation of the 2D materials but also provides a new approach to deriving information of edge orientations of mechanically exfoliated 2D materials by data mining of their macroscopic geometric features.

A Novel Self-locked Tube System for Energy Absorption

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ABSTRACT

Thin-walled round tubes are widely used in impact protection due to its low cost and high energy absorption. However, round tube system requires internal connections and boundary constraints to suppress the lateral splashing of tubes. Complicated constraints can increase installation time and thus make round tube system unsuitable for emergent protection. To break this limitation, a novel self-locked tube system is proposed [1]. The proposed system is composed of dumbbell-shaped self-locked tubes. When subjected to lateral impact, the dumbbell-shaped tubes can mesh with each other and thus provide lateral constraints to prevent lateral splashing. Therefore, the self-locked system can work immediately after the tubes are put together, with no need of any internal connections or boundary constraints. The self-locking effect of the proposed system is validated by impact experiments and finite element method (FEM) simulations. A plastic hinge model is developed to estimate the energy absorbing properties of the single self-lock tube [2], which is validated by both FEM simulation and experiments. Based on the theoretical analysis, the effects of geometry of the tube on energy absorption are studied and the optimal geometry design of the tube is discussed. Besides, the stacking arrangement of the multiple-tube system is investigated by FEM simulations, and a general guideline on the structural design of proposed multiple-tube system is provided. Furthermore, an internally nested self-locked tube system is proposed to improve the energy absorption capacity [3]. The basic unit is a dumbbell-shaped tube nested by round tubes inside, and is investigated by plastic hinge model, experiment and FEM simulation. The geometric parameters of inner tubes are investigated, and suggestions on designing an internally nested self-locked tube system are provided. References: [1] Chen Y., Qiao C., Qiu X., Zhao S., Zhen C., Liu B., A novel self-locked energy absorbing system, *Journal of the Mechanics & Physics of Solids*, 87 (2016) 130-149. [2] Qiao C., Chen Y., Wang S., Yang K., Qiu X., Theoretical analysis on the collapse of dumbbell-shaped tubes, *International Journal of Mechanical Sciences*, 123 (2017) 20-33. [3] Yang K., Chen Y., Liu S., Qiao C., Yang J., Internally nested self-locked tube system for energy absorption, *Thin-Walled Structures*, 119 (2017).

Finite Element Simulation of Metallic Sandwich Plates with Graded Lattice Cores Subjected to Blast Loading

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ABSTRACT

Sandwich plates with cellular cores have been increasingly exploited as explosion protection structures [1]. Among a number of cellular cores, lattice truss core structure has been identified as one of the most promising candidates for ultra-lightweight core constructions due to its open topological configuration and more controllable optimization design process [2]. To further enhance the blast resistance of sandwich structures, graded lattice truss cores, where the relative density of cores itself vary layer-by-layer, can be utilized in sandwich structures. Due to the superior core compression and the wave dissipation characteristics of the graded core layers, the energy absorption capability of core layers and the blast resistance of the sandwich structure can be improved. In this research, 3D finite element simulations of metallic sandwich plates with graded lattice truss cores under blast loading have been carried out using the ABAQUS/Explicit software. The applied impulsive pressure distribution on the surface of the plates was calculated using the CONWEP code. The relative density of core layer was regulated to vary with sectional dimension of core truss members. The panels were made of stainless steel AL6XN which was assumed to follow bilinear strain hardening and strain rate-dependence. It is observed that the blast resistance capability of sandwich plates was sensitive to graded arrangement of the core relative density. The graded sandwich plates would exhibit a better blast resistance than the ungraded ones. Keywords: graded lattice cores; sandwich plates; finite element simulation; blast resistance

Investigation on Mechanical Properties and Memory Shape Effect of CNT-Reinforced SMP by Using MD Simulation

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ABSTRACT

Shape memory polymers (SMPs) are promising smart materials that can recover their original shape upon exposure to external stimuli from temporary shape. It offers wide potential applications due to unique shape-changing functionality. However, SMPs with high mechanical strength are increasingly needed. The reinforcement mechanism of nano inclusions on the mechanical properties of nanocomposites is still a controversial issue. In this work, physical and mechanical properties of polyethylene (PE) polymer nanocomposites infusing different content of single-walled-carbon-nanotube (SWNT) were investigated by molecular dynamics (MD) simulations. The effect of nano inclusions on primitive chain network of PE matrices was also considered. It is found that mean squared displacement of the PE matrix infused with SWNT junction is smaller than that of pure PE. However, these nano inclusions did not significantly alter the underlying mesh of primitive chain network of PE matrices. The change of mechanical properties associated with these nano inclusions should be directly attributed to the interaction between polymer matrices and nano inclusions. For this purpose, we carried out the analysis on the thermodynamic cycle of the shape memory polymer at different tensile strain, and obtained the effect of the various content of SWNT on the mechanical properties of the SCNT/PE composites. The effect of nanofiller dispersion on the glass transition temperature of the nanocomposites was studied. The stress-strain relationship under uniaxial tension at different temperatures were obtained, which demonstrates the mechanical properties at different phases. These results illustrate the mechanism of shape memory effect and recovery in amorphous polymers.

Structural Analyses with Explicit Considerations of Microscopic Damage Evolution for Virtual Testing of Composites

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ABSTRACT

The rapid advances in novel computational mechanics theories, computing power, coupled with ultra-high resolution experimental characterization for interior progressive damage processes in structural materials, are enabling a new paradigm for rapid invention of new structural materials with novel microstructures for multifunctional applications. This method advocates a comprehensive multi-scale approach that utilizes a system of hierarchical models, engineering tests, and specialized laboratory experiments. To achieve practical applications of such methods in routine engineering design processes, these methods have to demonstrate that they can faithfully assess the safety and durability of a structure that is subjected to the intended loading environment during its entire lifespan. However, it is inevitable that the majority of engineering materials exhibit progressive damage evolution during their lifetime. In a typical composite structure, the progressive damage evolution process involves the initiation of numerous discrete, small cracks at locations that cannot be predetermined, their coupled evolution with local delamination to form one or several major cracks of structural criticality, which lead to the catastrophic structural failure. It is thus critical to be able to explicitly account for the progressive evolution of all major types of discrete damage events with high fidelity in a structural model. In this paper, we extend a recently developed method named augmented finite element method (A-FEM), which can account for arbitrary multiple cracking events in composites with orders of magnitude improve in numerical efficiency and accuracy, to explicitly include damage accumulation descriptions of various damage modes in composites (i.e., matrix cracking, fiber rupture in tension/kinking in compression, and delamination) under general thermal-mechanical loading. It will be demonstrated with ample validated examples that the A-FEM based simulation platform is able to predict key structural performance characteristics for structural design engineers, including the static strength, strength degradation under thermal-mechanical cyclic loading, the influence of temperature history to the static and fatigue strength, and more importantly, the probability of structural failure at any loading history. A rigorous multiscale validation procedure involving standard engineering tests for macroscopic quantification and in-situ micro-CT for tracing internal damage accumulation in real materials will also be included to promote further discussions on how to assess the credibility of simulated results.

A Reproducing Kernel Finite Volume Method

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ABSTRACT

Meshfree methods have evolved into a powerful technique for solving challenging scientific and engineering problems where traditional methods fall short. However, several treatments are required to obtain an efficient, stable, and convergent Galerkin implementation [1], and enforcement of essential boundary conditions is non-trivial [2]. On the other hand, strong-form collocation meshfree methods do not suffer from these issues, yet require expensive higher order derivatives, and in order to converge many collocation points must be employed [3]. This work introduces a reproducing kernel finite volume method. A particular weight function is selected which leads to a set of collocation equations, and offers ease of implementation, and an efficient nodal collocation-type method which does not require higher order derivatives. The formulation automatically satisfies the Variational Consistency conditions, and gives optimal convergence without special treatment. No unstable modes are observed, and thus apparently the method also offers stability without additional techniques. Finally, the essential boundary conditions are directly enforced, which leads to additional ease of implementation. The method is developed for elastostatics and elastodynamics, and several benchmark problems are solved to show its effectiveness in terms of stability, accuracy, and efficiency. 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] S. Fernández-Méndez, A. Huerta, "Imposing essential boundary conditions in mesh-free methods," *Comput. Methods Appl. Mech. Eng.* (193) 12, 1257–1275, 2004. [3] H.-Y. Hu, C.-K. Lai, J.-S. Chen, "A study on convergence and complexity of reproducing kernel collocation method," *Interact. Multiscale Mech.* (2) 3, 295–319, 2009.

Thermomechanical Multiscale Modeling of Boron Nitride Reinforced Nanocomposites

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ABSTRACT

Boron nitride (BN) has promising mechanical, dielectric and thermal transport properties comparable to graphene and carbon nanotube (CNT) with greater thermal stability than the two nanocarbon structure. Moreover, BN has excellent radiation shielding characteristics which makes it a good reinforcement for deep space polymer nanocomposites. The BN has two representative forms of BN nanosheet and BN nanotube (BNNT) each of which has exactly same configuration to the graphene and CNT respectively. Therefore, BN reinforced nanocomposites can be modeled as infinite cylinder type or penny shaped inclusion type inclusion problem in micromechanics model. Since characteristics length scale of BN nanosheet and BNNT are in nanometer scale, molecular modeling and simulation of BNT reinforced nanocomposites representative volume element (RVE) can also be addressed in analysis and design of nanocomposites. In this presentation, the thermomechanical properties of BN reinforced nanocomposites are determined from classical molecular dynamics (MD) simulations. In MD simulations, nanocomposites RVEs consisting of single BN and amorphous polymer matrix are constructed and elastic and thermal properties are determined according to the volume fraction of BN. Once thermomechanical properties of BN, polymer, and BN nanocomposites are determined, interface condition between BN and polymer matrix are characterized by means of inverse multiscale modeling approach or BN/polymer laminated interface molecular structures. Since interfacial sliding or phonon scattering are of primary importance for the effective load transport or thermal energy transport, a micromechanics model which can describe these interfacial properties are developed from conventional micromechanics models. Once the thermomechanical multiscale modeling framework is completed, some validation studies are performed to evaluate the accuracy and efficiency of the proposed model by comparing with experimental results or MD simulation results.

Influence of Delay and Noise on the Stability of Periodic Attractor in Nonlinear Vibration Isolator

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ABSTRACT

In this paper, we present a detailed study of time-delayed feedback control of the quasi-zero-stiffness SD (smooth and discontinuous) oscillator driven by stochastic environmental fluctuations. This oscillator is composed of a lumped mass connected with a vertical spring and a pair of horizontally springs, which can achieve the quasi-zero-stiffness widely used in vibration isolation. We investigate the effects of time-delayed control force and nonlinear damping on the mean first passage time from the periodic attractors to reveal the complicated nonlinear stochastic dynamics of this system. Varying the intensities of noise sources, it is possible to analyze the behavior of the switching time from the unstable periodic attractor to the stable one in different delay regimes. Moreover, the optimum time delay is obtained based on the consideration for the phenomena of noise- and delay-enhanced stability. Finally, a quantitative measure for amplitude response has been carried out to evaluate the isolation performance of the controlled system. This paper established the relationship between the parameters and vibration properties of the damping and stiffness nonlinearities SD oscillator which provides the guidance for optimizing time-delayed control for vibration isolation of the nonlinear systems.

Optimizing Battery Design Using Multifidelity Model

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ABSTRACT

We develop a mathematical framework to study the optimal design of air electrode microstructures for lithium-oxygen (Li-O₂) batteries. The design parameters to characterize an air-electrode microstructure include the porosity, surface-to-volume ratio, and parameters associated with the pore-size distribution. A surrogate model for discharge capacity is first constructed as a function of these design parameters. In particular, a Gaussian process regression method, co-kriging, is employed due to its accuracy and efficiency in predicting high-dimensional responses from a combination of multifidelity data. Specifically, a small sample of data from high-fidelity simulations are combined with a large sample of data obtained from computationally efficient low-fidelity simulations. The high-fidelity simulation is based on a multiscale modeling approach that couples the microscale while the low-fidelity simulation is based on an empirical macroscale model. The constructed response surface provides quantitative understanding and prediction about how air electrode microstructures affect the discharge capacity of Li-O₂ batteries. The succeeding sensitivity analysis via Sobol indexes and optimization via genetic algorithm offer reliable guidance on the optimal design of air electrode microstructures.

An Enhanced Generalized Algorithm for Finite Particle Method

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ABSTRACT

Finite Particle Method (FPM) is a significant improvement to the traditional SPH method, which can greatly improve the computational accuracy for the whole computational domain, including both interior area and boundary area. However, long computational time is always a big obstacle to the development of FPM, which is caused by the large amount of calculation on solving the linear equations for each particle in the computational domain. Therefore, how to obtain a higher computational accuracy in the limited computational expense is becoming more and more attentive. Based on our previous Specified FPM (SFPM) algorithm, a developed generalized FPM method (GFPM) is derived, which introduces the additional information of the Taylor remainder into the calculation of traditional FPM. Then by combining the FPM and GFPM, an enhanced generalized Finite Particle Method (EGFPM) is proposed. Numerical results show that, (1) the function and the derivative values calculated by EGFPM obtain an improvement of about three-order of magnitude and one-order of magnitude over FPM respectively. (2) For a given computational accuracy, EGFPM needs fewer particles distributed in the computational domain than FPM. (3) The computational time by EGFPM show just slight longer than FPM, and the time difference is just average 4‰ of traditional FPM.

The Molecular Dynamics Simulation on Mechanical Properties of Y₂O₃/Ni Composites

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ABSTRACT

Molecular dynamics (MD) simulations were carried out to investigate the influence of Y₂O₃ contents and dispersity on the mechanical properties of Y₂O₃/Ni composites. The well-dispersed addition of 1.0wt%, 2.0wt%, 3.0wt%, 4.0wt%, 5.0wt%, 6.0wt% Y₂O₃ to Ni matrix are studied, whose results show the 2.0wt% Y₂O₃/Ni composite provides the best Young's modulus and bulk modulus when Y₂O₃ disperses uniformly in the Ni matrix. Shear modulus of the composites reaches the highest at the content of Y₂O₃ being 3.0wt% while 2.0wt%Y₂O₃/Ni composite has the nearly same value of shear modulus with 3.0wt%Y₂O₃/Ni (78.2672GPa and 78.3469GPa respectively). The influence of dispersity on Y₂O₃/Ni composites was also studied by MD simulation, which indicates the aggregation of Y₂O₃ causes a sharp decline on both Young's modulus and shear modulus. A series of experiments were also carried out to test the MD simulations. Mechanical alloying (MA) and Spark Plasma Sintering (SPS) were adopted to produce the Y₂O₃/Ni composites with the content of Y₂O₃ being 1.0wt%, 2.0wt%, 3.0wt%, 5.0wt%. XRD, SEM and compressive tests were taken to analyze the properties of the developed composites. SEM results indicate the appearance of aggregation occurs in the composites with the addition of Y₂O₃ above 2.0wt%, which leads to a sharp decrease in mechanical properties, as the same as the MD simulation results. Compared with previous researches done by W Chen et al[2] whose results show the most appropriate Y₂O₃ content is 1.5wt% due to the poor dispersion of Y₂O₃, the present experimental study shows a larger proper Y₂O₃ content (2.0wt%) which is consistent with the MD simulations. References: [1] J.D. Giallonardo, U. Erb, K.T. Aust, et al. The Influence of Grain Size and Texture on the Young's Modulus of Nanocrystalline Nickel and Nickel-iron Alloys[J]. Philosophical Magazine, 2011, 91(36):4594-4605. [2] Chen W, Xiong W, Zhang X. Effect of Y₂O₃ Content and Sintering Temperature on Mechanical Properties of ODS Nickel-Based Superalloy[J]. Rare Metal Materials & Engineering, 2010, 39(1):112-116.

Identification of Bridge Modal Properties from the Contact-point Response of a Moving Test Vehicle

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ABSTRACT

The response of the contact point of the vehicle with the bridge, rather than the vehicle itself, is firstly proposed for modal identification of bridges by a moving test vehicle. To begin, approximate closed-form solutions were derived for the vehicle and contact-point responses, and verified by finite element solutions. The contact-point acceleration is born to be free of the vehicle frequency, an annoying effect that may overshadow the bridge frequencies in case of rough surface. From the frequency response function (FRF) of the vehicle with respect to the contact point, it was shown that the contact-point response generally outperforms the vehicle response in extracting the bridge frequencies in that more frequencies can be identified. In the numerical simulations, the contact-point response was compared with the vehicle response for various scenarios. It is concluded that in each case, say, for varying vehicle speeds or frequencies, for smooth or rough road surfaces, with or without existing traffic, the contact-point response outperforms the vehicle response in extracting either the frequencies or mode shapes of the bridge.

A Triple-scale Asymptotic Homogenization for Coupled Conduction-radiation Problems in Porous Materials with Multi-level Configurations

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ABSTRACT

The novelty of the newly method developed is by implementation on heat conduction-radiation problems in porous materials with multiple heterogeneities. The heterogeneities of porous structures are considered by periodic layouts of unit cells on the microscale and mesoscale. A new micro-meso-macro formula based on reiterated homogenization methods and multiscale asymptotic expansions is established. The equivalent coefficients are obtained by up-scaling procedure and homogenized problem are derived. In this method, both the mesoscopic and microscopic information is combined with homogenization solution to catch local oscillation inside the material. The numerical results show that the three-scale asymptotic expansion proposed in this manuscript can be useful for determination of the heat transfer properties of porous materials and demonstrate its potential applications in engineering and technology.

Model Reduction of Parametrized Aerodynamic Flows: Adaptive Discontinuous-Galerkin Reduced-basis Empirical Quadrature Procedure

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ABSTRACT

We present a model reduction formulation for parametrized nonlinear partial differential equations (PDEs) with emphasis on steady aerodynamic flows modeled by the compressible Reynolds-averaged Navier-Stokes (RANS) equations. The approach builds on four key ingredients: the discontinuous Galerkin (DG) method which provides high-order accuracy and stability for convection-dominated flows; an anisotropic adaptive mesh refinement strategy which quantifies and efficiently controls the spatial finite-element discretization error; reduced basis (RB) spaces which provide rapidly convergent approximations to the parametric manifold; sparse empirical quadrature rules which provide "hyperreduction" to enable rapid evaluation of the nonlinear DG residual and output forms associated with the RB spaces. The quadrature rules are identified by a DG extension of a linear program (LP) empirical quadrature procedure (EQP) [1] which (i) admits efficient solution by a simplex method, (ii) guarantees energy stability, and (iii) directly controls the solution error induced by the approximate quadrature. The errors associated with the spatial discretization, reduced basis approximation, and hyperreduction are simultaneously controlled in a systematic and automated manner by a greedy algorithm in the offline stage. We demonstrate the approach for parametrized steady aerodynamic flows with variations in physical flow conditions or mathematical model parameters. The former enables rapid exploration of the design space. The latter enables combined model and discretization uncertainty quantification (UQ) of the RANS equations with the Spalart-Allmaras (SA) turbulence model, where the model error arises from the uncertainty in SA model parameters. In both scenarios, the DG-RB-EQP method achieves significant computational savings while tightly controlling the discretization error associated with the spatial, reduced basis, and quadrature approximations. The rapid predictions provided by the DG-RB-EQP method also enables control of the Monte Carlo (MC) sampling error in the context of UQ. [1] AT Patera and M Yano, An LP empirical quadrature procedure for parametrized functions, *Comptes Rendus Mathematique*, accepted.

Computational Studies on the Failure Problems in Lithium-ion Batteries

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ABSTRACT

Developing batteries with high capacity and long cycle life would not only be of significant value to industries but help alleviate pressure from energy shortage. High-capacity batteries require electrode materials with high capacity which, however, tend to be accompanied with large volume change during lithiation and delithiation process. For example, Silicon (Si), an anode material with the highest capacity, experiences 300-400% volume change during the charge/discharge processes. Such large volume change is the Achilles' heel of Si because it would cause a series of failure problems such as fracture of the electrode materials and delamination from current collector, resulting in loss of electric conductivity and capacity fading. In the past a few years, we have been studying, by using computational mechanics approaches, the lithiation-induced failure problems in a variety of anode materials including SnO₂ nanowires [1], carbon-coated silicon core-shell nanoparticles [2] and yolk-shell carbon-coated silicon nanoparticle [3]. Our results not only shed light on the mechanisms of these failure phenomena, but also provide guidance for alleviating or even solving the associated problems. References: 1. Q. Li, W. Li, Q. Feng, P. Wang, M. Mao, J. Liu, L.M. Zhou, H. Wang, H. Yao*, 2014. Thickness-dependent fracture of amorphous carbon coating on SnO₂ nanowire electrodes, *Carbon* 80, 793-798. 2. W. Li, K. Cao, H. Wang, J. Liu, L.M. Zhou, H. Yao*, 2016. Carbon coating may expedite the fracture of carbon-coated silicon core-shell nanoparticles during lithiation, *Nanoscale* 8, 5254-5259. 3. W. Li, Q. Wang, K. Cao, J. Tang, H. Wang, L.M. Zhou*, H. Yao*, 2016. Mechanics-based optimization of yolk-shell carbon-coated silicon nanoparticle as electrode materials for high-capacity lithium ion battery, *Composites Communications* 1, 1-5.

Stochastic Reconstruction of Complex Heavy Oil Molecules Using an Artificial Neural Network

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ABSTRACT

An approach for the stochastic reconstruction of petroleum fractions based on the joint use of artificial neural networks and genetic algorithms was developed. This hybrid approach reduced the time required for optimization of the composition of the petroleum fraction without sacrificing accuracy. A reasonable initial structural parameter set in the optimization space was determined using an artificial neural network. Then, the initial parameter set was optimized using a genetic algorithm. The simulations show that the time savings were between 62 and 74 percent for the samples used. This development is critical, considering that the characteristic time required for the optimization procedure is hours or even days for stochastic reconstruction. In addition, the stand-alone use of the artificial neural network step that produces instantaneous results may help where it is necessary to make quick decisions.

Effect of Boiling Point and Density Prediction Methods on Stochastic Reconstruction

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ABSTRACT

Stochastic Reconstruction (SR) methods are used to generate a series of molecules that mimic the properties of complex mixtures using partial analytical data. Determining a quantitative composition using these methods is limited by the property prediction methods used. This paper addresses the use of two key measurements in the characterization of petroleum fractions, namely, density and boiling point distributions. It is known that the different methods used in estimating these two basic properties have different error rates. Boiling point prediction performances of the various group contribution methods were tested by means of the molecular library established for the molecules that can be present in the petroleum fractions. It has been observed that the combined use of these methods causes about 50% smaller sum of squared errors than any method alone. The predictive performances of the density calculation methods were similarly tested. The best-calculated density results were found by the combination of the linear mixing rule based on molar fractions and the Yen - Woods method.

Contact along Virtual Interfaces for Wear Simulation: Coupling the X-FEM with the Mortar Discretization

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ABSTRACT

Interaction between solids involving contact, friction, adhesion and wear are complex both with regard to their mathematical description and numerical treatment. The interfacial nature of these phenomena lays a strong emphasis on the interface discretization scheme. Stability and appropriate patch-test performance of these schemes are necessary ingredients to ensure the overall accuracy and robustness of the contact treatment. A relative motion between contacting bodies can lead to material removal (wear) of rubbing solids. The change of geometry change the contact pressures, and thus leads to alteration of the system's global response and affects the further evolution of wear. Numerical simulation of wear usually involve (1) constitutive local wear laws determining the wear depth evolution at every effective cycle, (2) remeshing procedures to capture the shape changes at the interface, and (3) field remapping in case of material behavior involving internal variables. In this presentation we will suggest a novel method enabling to simplify the treatment of wear problems and ensuring optimal convergence as well as accurate representation of surface tractions, which is essential for wear simulation. Face-to-face discretization techniques combined with penalty-based or Lagrange-multiplier based treatment of contact/friction constraints form the state of the art methods enabling to handle contact interaction along non-conformal interfaces in a robust way and ensure the accuracy of surface tractions [1]. The extended finite element method (X-FEM) presents a different technique to handle intra-mesh discontinuities: shock waves, oxidation fronts, composite materials, voids and cracks [2]. Combining the face-to-face contact formulation with the X-FEM method presents an attractive option to treat contact problems along virtual surfaces/interfaces with incompatible meshes: the face-to-face discretization ensures an accurate treatment of contact and the X-FEM ensures independence of interfaces of the finite element mesh. The virtual contact surface embedded in the volumetric mesh can incorporate geometrical aspects, such as roughness, and can evolve in time due to wear and/or third body accumulation. The main aspects of such a coupling between the mortar and the X-FEM methods will be presented as well as a few examples. [1] M. Gitterle, A. Popp, M. W. Gee, and W. A. Wall (2010). Finite deformation frictional mortar contact using a semi-smooth newton method with consistent linearization. *Int J Num Methods Eng*, 84(5):543-571. [2] N. Sukumar, D.L. Chopp, N. Moës, and T. Belytschko (2001). Modeling holes and inclusions by level sets in the extended finite-element method. *Comp Methods Appl Mech Eng*, 190(46):6183-6200.

Trend of Patents about Utilization of AI Technology in Extended Computer Aided Engineering Region ~ The Field of Application and the Proposal of Development Policy of AI Technology in Manufacturing Industry ~

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ABSTRACT

These days, the third generation AI technology characterized by deep machine learning is developing rapidly and it is widely utilized in various industrial fields, for example image recognition and automatic driving etc. CAE (Computer Aided Engineering) technology has been quite important for the design and development of new products and ecosystems in the enterprises. However the AI technology is not yet widely available for the Working-Level design process in the manufacturing industry. In this paper, the patent trends of AI technology about "Extended CAE" are described. First, a concept of "Extended CAE" in the industrial manufacturing process is defined. Next, the patent trends of AI technology about the Extended CAE for manufacturing industry about (1) an automated production in a factory, (2) high efficiency operation in a construction site and (3) semi-automated patent search and application are mentioned. Finally, the future development plans of AI technology about industrial manufacturing process in the enterprises are proposed.

Finite Strain Meshfree Co-rotational Formulation for Hyperelastic Solids

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ABSTRACT

Prior research in finite element analysis with incompressible materials has established improved performance when the analysis is placed within a co-rotational formulation. The present work aims to show that these benefits also transfer to the meshfree setting. In this work a finite strain meshfree formulation is included within a co-rotational framework, which to our knowledge has not been done heretofore. Advantage is taken of the close relation between local engineering strains and Biot strains (advocated by Crisfield [1], Moita [2]) in the refined nodal discretization limit. Under such conditions individual nodal stresses approach a state of homogeneous local stress. Biot stresses and strains allow the incorporation of finite strains and hyperelastic material models. For the meshfree formulation, any set of meshfree basis functions is suitable; herein, we adopt maximum-entropy basis functions (Yaw et al [3]). Nodal integration over a Voronoi cell background with stabilization is employed. The formulation passes the large strain patch test for the case of pure shear. Results for plane stress stretched membrane, plane strain axial extrusion, and Cook's membrane are among the benchmark problems presented. We will conclude with the promise and outlook of finite strain meshfree-based co-rotational formulations. [1] M. A., Crisfield. *Non-linear Finite Element Analysis of Solids and Structures – Vol 2 Advanced Topics*. John Wiley & Sons Ltd., Chichester, England, 1997. [2] G. F., Moita. "Non-linear finite element analysis of continua with emphasis on hyperelasticity", Ph.D. Thesis, Imperial College, London, 1994. [3] L. L. Yaw, N. Sukumar, and S. K. Kunnath. Meshfree co-rotational formulation for two-dimensional continua. *International Journal for Numerical Methods in Engineering*, 79(8):979–1003, 2009.

Electric Field-Induced Adjustable Mechanical Property and Deformation Behavior of Fluid-Filled Carbon Nanotubes

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ABSTRACT

Water-filled carbon nanotubes (CNTs) have been successfully fabricated and separated in laboratory. It has also been demonstrated that the ions could enter the CNTs spontaneously. Hence, it is possible to further fabricate the salt water-filled CNTs based on the present experimental technology. As an ideal candidates for structural elements or functional components in nanoscale systems, the CNTs are expected to be accurately and conveniently controlled, including their mechanical property, deformation and so on, which has great potential applications in micro-electro-mechanical systems, microfluidic chips, etc. Due to the sensitivity of polar water molecules and ions to electric field, the controllable performance may be feasible for fluid-filled CNTs. In this report, the systematic study on the mechanical property and deformation response of pure water and salt water-filled CNTs under the electric field are presented, including the compression test, torsion deformation, size dependence, pre-strained effect, controllable tension and bending, etc. For the water-filled CNTs, the results based on the molecular dynamics (MD) simulations indicate that the mechanical properties (the elastic modulus, Poisson's ratio, critical buckling stress) would vary with the electric field intensity, which exhibit a nonlinear dependence on the diameter of CNTs. As for the salt water-filled CNTs, the electric field could result in the tension and bending deformations. Some theoretical models are also constructed to verify the deformation behavior of the fluid-filled CNTs. Furthermore, the mentioned controllable performances are also utilized to design molecular sieving and nanoscale trigger. The present research reveals the adjustable 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 (Nos. 11672063, 11672062, 11772082, 11472117 and 11232003), the 111 Project (No. B08014), Young Science and Technology Star Program of Dalian (2016RQ018) and Fundamental Research Funds for the Central Universities are gratefully acknowledged.

Extended Level Set Methods (X-LSM) for Shape and Topology Optimization on Manifolds

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ABSTRACT

The level-set-based topology optimization (TO) approach has been considered as a powerful tool in generating innovative designs. However, the conventional level set functions are defined in the Euclidean space (R^2 and R^3), which cannot satisfy the demand of TO on general freeform surfaces. In this paper, we propose a new method to address the problem of structural shape and topology optimization on free-form surfaces which is mathematically defined as manifolds. By using conformal parameterization, we extend the level set based topology optimization framework from the Euclidean space (R^2 and R^3) to surfaces with arbitrary topologies. In our method, a manifold is conformally mapped onto a 2D rectangular domain, where the level set functions are defined afterward. We prove that by using this conformal mapping, the corresponding covariant derivatives on a manifold can be represented by the Euclidean differential operators after a scalar multiplication. Therefore, the topology optimization problem on free-form surfaces can be formulated as a 2D problem in the Euclidean space. To update the level set function, we can define and solve a new set of partial differential equations (PDEs), including the modified Hamilton-Jacobi Equation in 2D instead of on the free-form surface. Compared with other established approaches which need to project the Euclidean differential operators to the surface, the computational difficulty of the X-Level Set method is highly reduced. In addition, the conformal mapping between the free-form surfaces and the 2D domain is an explicit approach. Moreover, it is intuitive to observe the design revolution on the manifold. Two benchmark examples of the mean compliance topology optimization problems on free-form shell structures are studied, and the optimized solutions are presented to demonstrate the validity and effectiveness of the proposed method.

Coupled Physics Simulation of Fracture in Nuclear Fuel Pellets Induced by Resistive Heating

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ABSTRACT

Nuclear light water reactors (LWRs), which make up the majority of the commercial power reactors currently in use worldwide, use ceramic uranium oxide fuel pellets stacked within long cylindrical metallic fuel rods. During normal operation, these fuel pellets experience significant gradients in temperature, and as a result, corresponding high stresses induced by nonuniform thermal expansion. This causes the fuel pellets to fracture very early in their service life. While this fracturing is not a direct safety concern, it does significantly affect a number of aspects of the performance of the nuclear fuel system. There are ongoing efforts to base the material behavior models used for LWR fuel performance on physical behavior rather than on empirical models that represent those effects indirectly. To that end, capabilities have been added to the BISON nuclear fuel performance code developed at Idaho National Laboratory to use several techniques for modeling fracture within multiphysics fuel performance models. These techniques include the extended finite element method (XFEM), smeared cracking, and peridynamics. As these fracture models have matured, the need for validation data has become clear. Because it is extremely difficult to monitor the processes of fracture propagation within a nuclear reactor, separate-effects validation experiments of fracturing fuel outside the reactor, but under thermal conditions comparable to those seen in the reactor are being planned. One of these experiments employs the use of resistive heating by applying a current through a fuel pellet to obtain volumetric heating similar to that provided by fission processes in the nuclear reactor. This is expected to produce temperatures that are much higher on the inside of the pellet than on the outside, and which will result in thermally-induced cracking similar to that observed under normal LWR operation conditions. The BISON code is an inherently multiphysics simulation environment, and has been extended to model electrical fields coupled with the thermal and mechanical fields typically simulated in that tool. With this added capability, it is being used to simulate fracture induced by an electric current applied to a pellet. This is being used to guide the development of these validation experiments, and the outcomes of those tests will be used to improve the accuracy of the models for fracture in BISON. This talk will describe the coupled physics models, the solution methods used, and show the results of their application to this problem.

Modelling of landslides with the Material Point Method

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ABSTRACT

Landslides and slope instabilities represent one of the most important problems in geotechnics and cause significant damage to properties as well as human life around the world. Understanding the mechanics of the slope deformation process is of particular importance for risk assessment. Traditionally, most geotechnical analyses focus on failure prediction (i.e. onset of failure); however, despite the probability of failure at the initiation stage of a landslide is often small, it is essential to understand the post-failure behavior in order to minimize the risk of catastrophic damages. Hence, there is an urgent need to develop numerical schemes capable of simulating failure initiation and post-failure dynamics of landslides in a unique framework. In this work, the Material Point Method (MPM) is presented as a numerical technique capable of modelling large deformation problems and interaction between different materials. MPM discretizes the continuum into a set of material points that represent and move attached to the material, while main governing equations are solved at the nodes of a background computational mesh. With this dual description of the media, MPM can deal with large deformations of history-dependent materials without limitations of mesh tangling, and contact between different bodies is automatically solved. During the last decade, MPM has been applied to different engineering fields such as ice dynamics and fracture of wood, and recently it has received increasing attention in the geotechnical field, in particular in the analysis of landslides. In this work, different theoretical and real cases will be discussed in order to present the capabilities of MPM to analyze complex landsliding problems. Special emphasis will be dedicated to examine the Oso Landslide, which occurred in the State of Washington, USA on 22 March 2014. The Oso Landslide is one of the worst landslide disasters in the US history with 43 fatalities. It took place in multiple failure stages, travelled nearly 1 km over the floodplain involving several failure surfaces and significant soil softening.

The Elastic-Plastic Decomposition of Crystal Deformation at the Micro-nano Scale

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ABSTRACT

With the development of computer performance, it has become very popular to make use of molecular dynamics simulation to study mechanical properties of materials at micro-nano scales. From the instantaneous positions of atoms, some macroscopic mechanical properties of materials, such as the elastic constants, can be calculated. The usual procedure is as follows: firstly, taking the snapshots of an atomistic system at two different instants, the total deformation gradient can be evaluated by piecewise polynomial interpolation. However, the elastic and plastic deformation gradients can't directly obtained from the total deformation gradient. Thus, some predecessors extended the multiplicative decomposition of the total deformation gradients to the micro-nano scale, and developed some decomposition methods, which make success in some extent. But there are still some flaws in dealing with the atomic locations after unloading. Therefore it is necessary to develop a new decomposition algorithm on the elastic and plastic deformation gradients from total deformation gradient. In this paper, we develop a new algorithm to calculate the post-unloading configurations based on the fact that unloaded materials should be on a stable state, that is, the internal atomic arrangement of materials correspond with atomic locations of minimum total potential energy. Our algorithm is to decompose the total deformation gradient field into the elastic deformation gradient field and the plastic deformation gradient field, where the elastic deformation gradient comes from the microscopic lattice structure of unloading configurations retaining defects. Our algorithm successfully solves the flaws of the previous methods. And it is the basis for further studying the elastic-plastic properties based on MD simulation. The framework of this paper is as follows: first part is to point out the necessary of developing a new decomposition algorithm, and introduce the high order deformation elements based on the BCC/FCC lattice to calculate the total deformation gradient field. The second is to devote to the algorithm of obtaining post-unloading configurations, and the new decomposition algorithm. Final part is an example on tensed nanowire to verify the correctness of our algorithm.

N-S Equations and Relativistic Structures and Engineering Applications

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ABSTRACT

In this talk, we propose a novel fluid mechanics calculation method and the universality of asymmetric energy, and manufacture an asymmetric energy engine. Mechanics calculation: It is proposed that eddy currents and turbulent flows are infinite multi-scale vortex flow states defined as a point state, the logarithm-based logarithm of the non-dimensional quantities and the three logarithmically invariant circular log-dynamic equations are established, , For a variety of high-power polynomials formed by the state of flow, for concise, self-consistent, accurate solution. Engineering Application: Propose the principle and mechanism of asymmetric super-energy engine to solve the design and manufacture of long vortex vane and super-symmetric heat engine controlled by six programs. Manufacture of asymmetric super-engine, won the Chinese national invention patents: (1), Macro-type: positive and reverse flow can produce asymmetric transformers. That is, a fuel-free engine that is used to generate electricity. Project: "eccentric rotation engine", a small batch production. If the meeting allows, can bring to the show. (2), The concept of medium-sized: high and low heat can transform asymmetric super energy, resulting in 10 to 20 times more than traditional internal combustion engine, for transportation, power generation. Project: "a two-way vortex air-cooled negative pressure aerodynamic hydrogen engine" (ZL201410052227.0); "double-scroll negative pressure internal combustion engine" (ZL201510187088.7). (3) , Micro-type: The asymmetric super-energy is generated by the positive and negative nuclear energy conversion controlled by six programs. The project is "Small Safety and Environmental Protection Nuclear Power Engine".

Anisotropy of Microstructure in Compacted Granular Solids

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ABSTRACT

Compaction is one of the most common industrial processes used to achieve densification of powders and to develop tensile strength or resistance to crushing. Several factors, including powder properties, applied compaction pressure, and the shape of tooling affect the compaction process itself and the final microstructure. Even though several prior studies have addressed this topic in detail, the compaction process is still not well understood, particularly in terms of developing a mechanistic relationship between particle scale properties and the powder compact properties such as relative density and tensile strength. In order to understand the effect of particle properties, such as particle size, plasticity, elasticity, and surface bonding energy, on the powder compact, we ran several experiments and discrete particle simulations. We studied commonly used excipients for pharmaceutical products and metallic powders. The exact particle size distributions of the powders are represented in the simulations, and the mechanical properties of the particles are calibrated using the powder compaction experiment results. Then, we validated our simulation results based on experimental indirect tensile strength test. We found that the simulation results are quantitatively similar to experimental results. Once the simulations are validated, we used the simulations to investigate the microstructure evolution during the compaction process and the effect of particle properties, particularly that of the size and the mechanical properties of the particles. In this presentation, we will discuss the experimental and simulation methods and results in detail.

Evaluation of Dynamic Impact Analysis on Curved Surface Structure Using Isogeometric Elements

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ABSTRACT

In recent years, the model that can be handled by CAE (Computer Aided Engineering) is also complicated due to rapid improvement in computer performance, and the number of divisions of elements is also enormous, so the problem increasing the time required for the whole analysis due to the complication of the target in performing the analysis, the time taken to mesh the CAD (Computer Aided Design) model occupies most of the time of the whole analysis. Isogeometric analysis method was proposed to solve this problem. Isogeometric analysis is different from conventional FEM (Finite Element Method) analysis and it can be applied to CAD by using B-spline / NURBS (Non Uniform Rational B-Spline) basis function as shape function it is possible to use the created model directly for analysis, it is possible to shorten the time and improve the calculation accuracy. In this study, focusing on the high model reproducibility of the Isogeometric element, dynamic impact analysis of a structure having a curved surface was carried out and the performance of the Isogeometric element was evaluated. Impact analysis was performed dynamically using bonnet, door panel, etc. as a structure having a curved surface. In order to evaluate the performance of isotropic element, it was compared with the analysis result of a model made by ordinary finite element method. This study concludes, in order to verify the accuracy verification of the Isogeometric element and the FEM, we analyzed using a model with curved surface and comparative verification. Then we investigated the influence and analysis accuracy in dynamic collision analysis using Isogeometric element, and showed future prospects.

An Improved Extended Material Point Method for Crack Problems

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ABSTRACT

The extended material point method (XMPM)[1] has demonstrated its capabilities in the simulation of crack growth problems. Because of the use of the jump function as the enrichment function around the crack, the XMPM can describe the discontinuous displacement and velocities by only one set of background grid mesh. However, the jump enrichment function is unable to describe the crack tip direction and the crack length in the cell where the crack tip is located in. In this work, the asymptotic crack tip functions are used to enrich the nodes around the crack tip to make the XMPM able to simulate the crack direction and length in one cell. Naturally, the result around the crack tip and the prediction of the crack growth is more accurate. In addition, the original XMPM is based on the conventional MPM[2] framework. It also suffers the cell crossing noise. To deal with the above issue, we use one-point quadrature with the quadrature point located at the center of the element and the nodal velocity is obtained by the moving least squares method (MLS). This improved XMPM scheme needs additional handling at the boundary and the generalized interpolation material point (GIMP)[3] shape function is also used. Numerical examples show that the asymptotic crack tip enrichment function can make the XMPM give more accurate result around the crack tip than before. For a manufactured solution with large deformation, the use of one-point quadrature, MLS for the nodal velocity and the GIMP shape function show that the cell crossing noise is eliminated and the accuracy is much better. REFERENCES [1] Liang Y, Benedek T, Zhang X, et al. "Material point method with enriched shape function for crack problems[J]." *Computer Methods in Applied Mechanics and Engineering*, 2017, 322: 541-562. [2] Sulsky, Deborah, Zhen Chen, and Howard L. Schreyer. "A particle method for history-dependent materials." *Computer methods in applied mechanics and engineering* 118.1 (1994): 179-196. [3] S.G. Bardenhagen, E.M. Kober. "The generalized interpolation material point method." *Computer Modeling in Engineering and Sciences* 5 (6) (2004) 477–495.

Iron Ore Particle Production through Liquid CO₂ Penetration and High Pressure Gas Propulsion by CDEM (Continuous-Discontinuous Element Method)

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ABSTRACT

An average iron content of iron ore is less than 30%, rough crushing, fine crushing, milling and other processing must be executed before they can be smelted. Currently iron ore broken by mechanical grinding demands higher cost. We describe a novel methodology named CDEM (Continuous-Discontinuous element method), coupling finite element method and discrete element method, can accurately realize crack initiation, crack propagation based on porosity seepage model and block rupture model, which facilitate micron-sized iron ore particle production through liquid CO₂ penetration and high pressure gas propulsion. On the conditions of iron ore permeability coefficient, porosity and tensile strength test, a series of numerical experiments of iron ore powdering have been carried out under different initial pressure of the liquid CO₂ and different initial pressure of gas. The higher the initial pressure of gas, the higher the number of fine particles obtained. Together with the powdering experiments conclusion, we can provide theoretical guidance for industrialization of iron ore powdering. The liquid CO₂ penetration and high pressure gas propulsion method is much more environmentally friendly, efficient, energy saving, and effective.

Newly Optimized Silicene Interatomic Potential Model for Elastic Constants

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ABSTRACT

Silicene is the 2D structured silicon, which can be used as opto-electric devices such as FET due to the promising electrical properties [1]. However, silicene can be deformed by mechanical stress during fabrication or operation, and electric properties transition will be occurred. For this reason, research of correlation between stress and deformations would support to control the manufacture process or operation environments. Previous results of mechanical tests by molecular statics simulations in the elastic regime are not accorded with the results of DFT calculation. The reason of this outcome is induced by that most of interatomic potential models were developed to predict elastic behaviors of 3D structures. In this study, authors conducted parameter optimizations of Tersoff potential model in order to predict elastic constants consistent with DFT values, including Young's modulus, Poisson's ratio and Bending modulus [2]. REFERENCES [1] L. Tao et al.: Silicene field-effect transistors operating at room temperature, Nat. Nano., Vol.10, pp.227—231, 2015. [2] J. Tersoff, Phys. Rev. B, 37, 12, (1988) 6991–6999

Topology Optimization with Finite Element Based k-e Turbulent Model

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ABSTRACT

In this research, a new finite element (FE) based topology optimization (TO) for turbulent flow was developed using the k-e model, which is one of the Reynolds-Averaged Navier-Stokes (RANS) equations. Despite many innovative works on the subject of fluidic TO, it is still difficult to consider the impact of turbulent flow in TO. To consider the effect of complex turbulent fluid motion, this research considered the k-e finite element model. To conduct a successful TO, one issue is modification of the k-e turbulent model to account for topological evolution during the optimization process. To address this issue, we proposed the addition of penalization terms to the original governing equations. To show the validity of the present approach and the effect of turbulent flow on optimal layouts, some two dimensional benchmark designs studied for laminar flow were reconsidered. By considering the effect of turbulent flow, the eddy viscosity values were increased at some local regions due to the Boussinesq hypothesis, and naturally optimal layouts affected by the spatially varying viscosity were obtained in turbulent flow.

Molecular Dynamic study of Immobilization of the Laccase on Graphene Sheet

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ABSTRACT

Biofuel cells are the most anticipated future energy material. These biofuel cells get energy from the bio-material for variety of kinds. Many researchers have developed wearable biofuel cells that consumes the energy from the tears and blood [1]. These materials from our human body, contains enzymes that produce and accept electrons. Electron producing enzyme, especially the Glucose Oxidases are inserted in the anode of the fuel cell and Laccase that accepts electron are placed in cathode. Therefore, by the mechanism of the enzyme, biofuel cells are able to storage the electron then produce electricity as a battery. The most limitation of the biofuel cell is the power level. The power level of the fuel cells, have been progressed by enzyme immobilization methods. The most immobilization methods are the electrode modification of the biofuel cells. Carbon materials like graphene sheet or CNT are used because of good electric conductivity. These methods have been made remarkable progress to power level, but still, biofuel cells are not practical as other kind of ordinary batteries. In this paper, we conducted conformation and interaction studies of the Laccase in nano-scale with molecular dynamic simulation. As mentioned above, Laccase are the most well-used enzyme for the cathode that accepts the electron. Therefore, we have simulated molecular dynamics simulation with Laccase immobilized on graphene sheet. We then, analyzed conformation change of the laccase, graphene binding site, and the interaction energy between laccase and graphene sheet.

Multiscale and Multiphysics Integrated Simulations for Offshore Wind Farm Using K-Computer : An Overview

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ABSTRACT

An offshore wind farm for power generation consists of tens to hundred of large scale wind turbines. To promote the use of natural energy in Japan, the Japanese government has planned to develop wind farms generating totally 4 million kw of power by 2030. To do so, we need to take care of heavier weather conditions and narrower offshore sites in Japan, compared with European and US environments. To improve the performance of power generation of wind farms and the reliability of individual wind turbine, it is necessary not only to concentrate on the improvement of the individual wind turbine, but also to improve the accuracy of evaluating the degradation of power generation of wind turbine affected by wake interaction. Moreover, it is necessary to improve the reliability evaluation of individual wind turbine exposed to the wake. As a part of the post K-computer project (Flagship 2020 project), we have been developing multiscale and multiphysics integrated simulations for an entire offshore wind farm. The simulations consist of the following components, (a) Large-scale flow simulation of a wind farm taking into weather and terrain, (b) Large-scale LES simulation of two tandem wind turbines to evaluate an effect of wake into power generation taking into account multiscale phenomena in time and space domains such as atmospheric flow, wind turbine wake, turbine blade boundary layer, and (c) Flow induced vibration of wind turbine based on FSI simulation. In this presentation, we describe an overview of the simulation system.

Application of the Variational Phase Field Method to Hydraulic Fracturing: A Comparative Study

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ABSTRACT

The ability to predict complex hydraulic fracturing behaviour beyond conventional planar assumption in sub-surface e.g. in unconventional resources has been crucially important in order to understand and control the hydraulic fracturing process in the energy resource industry. Due to the complex boundary conditions and its multi-physical nature in sub-surface environments, modelling of hydraulic fracturing at a laboratory scale is difficult to extrapolate to a field scale. Among the many numerical techniques studied such as discrete element or extended finite element methods, an approach termed variational phase field model, which was originally proposed by Bourdin, Francfort and Marigo in 2000, has become increasingly popular within the hydraulic fracturing modelling community in the recent years. One of its strengths, the ability to handle complex un-prescribed crack paths, is a fundamental for the numerical simulation of hydraulic fracturing, and its unified formulation of fracture nucleation and propagation in any propagation mode with an arbitrary number of fractures is a very attractive feature of such a numerical implementation. From the original implementation of Bourdin et al., however, several adaptations are required for hydraulic fracturing applications, which are: 1) extension to porous media, 2) computation of fracture width, 3) coupling with fluid flow, and 4) compressive-tensile split of the strain energy for geo-materials. Thus, in this study, we focus our development on these points and compare how different phase-field formulations address these issues in somewhat different manners. Finally, we discuss our endeavour to improve the numerical efficiency in coupling of the multi-physical processes.

Personalized FEA of Femurs - A Leap to Clinical Practice

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ABSTRACT

Patient-specific CT-based high-order finite element models (p-FEMs) accurately predict ex-vivo experimental observations on human femurs, including risk of fracture [1,2]. They account for the exact geometry and inhomogeneous material properties, are created in a semi-automated manner from CT scans and validated on a large cohort of fresh frozen femurs. CT-based p-FEMs were applied to predict bone strength in patients with bone tumors to their femur [3], demonstrating excellent prediction capabilities. The first part of the talk addresses the methodology to semi-automatically generate the femur's FEM from CT scans, assign material properties, apply the stance position load and interpret the FE results according to surgeon's need. Application of FE methodology in clinical practice is subject to obstacles and surprises, however, at the same time is accompanied by tremendous satisfaction when it helps patients and saves pain and agony. The second part of the talk will address the steps undertaken to bring the methodology into clinical practice. We shall present two clinical studies for using our CT-based p-FEA: one related to the need of a prophylactic surgery of femurs with metastatic tumors and the other related to the risk of a contralateral fracture of the femur proximal part following fractures in the elderly population. Several cases analyzed during the clinical trials and the potential use of p-FEA in clinical practice will be presented. References: [1] N. Trabelsi et al. Patient-specific finite element analysis of the human femur - a double-blinded biomechanical validation. *J. Biomech.*, 44:1666-1672, 2011. [2] Z. Yosibash, et al. Predicting the yield of the proximal femur using high order finite element analysis with inhomogeneous orthotropic material properties. *Phyl. Tran. of the Roy Soc.: A*, 368:2707-2723, 2010. [3] Z. Yosibash, et al. Predicting the stiffness and strength of human femurs with realistic metastatic tumors. *Bone*, 69:180-190, 2014.

A Meshfree Quadrature Rule for Non-local Mechanics

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ABSTRACT

We present a meshfree quadrature rule for compactly supported non-local integro-differential equations (IDEs) with radial kernels. We apply this rule to develop a meshfree discretization of a peridynamic solid mechanics model that requires no background mesh. Existing discretizations of peridynamic models have been shown to exhibit a lack of asymptotic compatibility to the corresponding linearly elastic local solution. By posing the quadrature rule as an equality constrained least squares problem, we obtain asymptotic convergence by introducing polynomial reproduction constraints. Our approach naturally handles traction-free conditions, surface effects, and damage modelling for both static and dynamic problems. We demonstrate high-order convergence to the local theory by comparing to manufactured solutions and to cases with crack singularities for which an analytic solution is available. Finally, we verify the applicability of the approach to realistic problems by reproducing high-velocity impact results from the Kalthoff-Winkler experiments.

Mechanotransduction of a Vesicle Membrane and Its Implication in Cellular Mechanotransduction

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ABSTRACT

Mechanosensation is an important process in biological fluid–structure interaction. To understand the biophysics underlying mechanosensation, it is essential to quantify the correlation between membrane deformation, membrane tension, external fluid shear stress, and conformation of mechanosensitive (MS) channels. A multiscale continuum model is constructed for a MS channel gated by tension in a lipid bilayer membrane under stresses due to fluid flows. We illustrate that for typical physiological conditions vesicle hydrodynamics driven by a fluid flow may render the membrane tension sufficiently large to gate a MS channel open. In particular, we focus on the dynamic opening/closing of a MS channel in a vesicle membrane under a planar shear flow and a pressure-driven flow across a constriction channel. Our modeling and numerical simulation results quantify the critical flow strength or flow channel geometry for intracellular transport through a MS channel. The modeling and simulation (both boundary integral and dissipative particle dynamics simulations) results imply that for fluid flows that are physiologically relevant and realizable in microfluidic configurations stress-induced intra-cellular transport across the lipid membrane can be achieved by the gating of reconstituted MS channels, which can be useful for designing drug delivery in medical therapy and understanding complicated mechanotransduction. We then use this model to investigate the cellular mechanotransduction by primary cilia in the force-by-lipid paradigm.

A Simple A Posteriori Estimate on General Polytopal Meshes with Applications to Complex Porous Media Flows

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ABSTRACT

In this work we develop an a posteriori error estimate for lowest-order locally conservative methods on meshes consisting of general polytopal elements. We focus on the ease of implementation of the methodology based on H^1 -conforming potential reconstructions and $H(\text{div}, \Omega)$ -conforming flux reconstructions. In particular, the evaluation of our estimates for steady linear diffusion equations merely consists in some local matrix-vector multiplications, where, on each mesh element, the matrices are either directly inherited from the given numerical method, or easily constructed from the element geometry, while the vectors are the flux and potential values on the given element. We next extend our approach to steady nonlinear problems. We obtain a guaranteed upper bound on the total error in the fluxes that is still obtained by local matrix-vector multiplications, with the same element matrices as above. Moreover, the estimate holds true on any linearization and algebraic solver step and allows to distinguish the different error components. Finally, we apply this methodology to unsteady nonlinear coupled degenerate problems describing complex multiphase flows in porous media. Also here, on each step of the time-marching scheme, linearization procedure, and linear algebraic solver, the estimate takes the simple matrix-vector multiplication form and distinguishes the different error components. It leads to an easy-to-implement and fast-to-run adaptive algorithm with guaranteed overall precision, adaptive stopping criteria, and adaptive space and time mesh refinements. Numerous numerical experiments on practical problems in two and three space dimensions illustrate the performance of our methodology.

Inverse Transient Heat Flux Boundary Condition and Computation of Thermal Stress

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ABSTRACT

The structure can be sometimes affected by the high heat flux in real engineering, such as the high heat flux of spacecraft surface when it returns the atmosphere, but the high heat flux usually cannot be measured directly. A novel non-iterative inverse method based on the precise integration finite element method (PIFEM) is established for estimating the transient boundary conditions in this paper. First of all, we obtain the temperature of measured points by solving the direct problem based on PIFEM. After that, the matrices formed by the PIFEM need to be reassembled, and then the unknown transient heat flux of boundary can be obtained by the least-square method. Finally, we can use the inversed heat flux boundary condition to compute the temperature and thermal stress distributions of the structure by PIFEM. Numerical results show that the present method can obtain the great performance on the inversing accuracy, the computing efficiency is better than intelligent evolutionary algorithm, and the measured errors and the number of measured points have little effect on the inverse results.

Data-driven Reduced-order Modeling of Microvoid Evolution for Ductile Fracture

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ABSTRACT

Microvoid evolution plays an important role in the ductile fracture process. Although various Gurson-type models have been developed to account for microvoid morphology and distribution, as well as matrix hardening and plasticity anisotropy with considerable fitting parameters, it is difficult to derive a unified constitutive model that considers all of these parameters. This presentation introduces a data-driven reduced order computational homogenization method by explicitly modeling microvoid evolution for ductile fracture analysis. Instead of using a phenomenological constitutive law, the material behavior of each integration point in a macroscopic part is computed on-the-fly using a statistical volume element (SVE) with embedded microvoids and periodic boundary conditions. The matrix of the SVE is modeled with a single/poly crystal plasticity law which accounts for plastic flow anisotropy and creep. Microvoids are reconstructed to reflect the real material microstructure morphology and distribution. To simulate the fracture process within a reasonable computational time, we adopt a recently developed data-driven order reduction technique, called self-consistent clustering analysis (Liu, Z., Bessa, M.A. & Liu, W.K., 2016. *Computer Methods in Applied Mechanics and Engineering*, 306, pp.319–341.), for the SVE problem. The predicted void evolution in a SVE under uniaxial tension is validated by comparing with in-situ X-ray tomography observation of void-driven fracturing in an additively manufactured Nickel-based superalloy. Fracture toughness tests of a high strength steel using compact tension specimens are also simulated with the primary particles modeled using finite elements at the macroscale and secondary particles modeled in the microscale SVEs. The fracture toughness measurements and crack path are compared to experiments. The proposed method might be used for ultimate strength and fracture toughness optimization by controlling the microstructure.

High Performance Fully-Coupled Fluid-Solid-Acoustic Solver

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ABSTRACT

The evaluation of the acoustic perturbation with low Mach number in fluid-structure interactions is challenging. Due to the large discrepancy in time scale between the fluid and the acoustic behavior, the computational time is significantly increased if directly numerical simulation is to be used. In this talk, we will introduce an aeroacoustic model for nearly incompressible isentropic flows used in Navier-Stokes equations, which is then incorporated into a fluid-structure interaction framework to evaluate the impact of pressure fluctuation on a deformable solid. A finite element library, deal.II, is utilized to modularize the finite element program to solve the modified Navier-Stokes equations for the ease of modification of the parameters and increasing the overall performance of the computation. The fully-coupled fluid-solid-acoustic solver requires the linearization and optimization of an effective preconditioner. Test cases are performed to validate the computation performance and the accuracy of the presented model. As an application, we will present a vocal fold vibration simulation where fluid-solid-acoustic fields are coupled to simulate the acoustic fields produced by slightly compressible flow that interacts with the vocal fold tissues.

The Nacelle's Position Effect on Aerodynamics of Blended-Wing-Body Airplane

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ABSTRACT

The Blended-Wing-Body (BWB) airplane concept represents a potential revolution in subsonic transport efficiency for large airplanes[1]. Except the Wing-Body blended way, the propulsion airframe integration of BWB airplane also takes a very important role for its good aerodynamic performances. The wing engine mounting distorts lift distribution may creating poor cruise aerodynamics. Therefore, its need to be minimized through careful propulsion airframe integration design[2]. The nacelle's position effect on aerodynamics of Blended-Wing-Body airplane is analyzed in this paper. First, the aerodynamics of clean BWB configuration (wing-body without nacelle) and with nacelle's initial configuration are compared to get an idea of nacelle's effect on the wing-body's aerodynamics. Then, the nacelle at different positions effect on aerodynamics of wing-body are analyzed to see the nacelle's position effect on the wing-body's aerodynamics. And moreover, the wing-body's effect to nacelle's aerodynamics is also compared. The initial model of 300 seating civil BWB airplane is shown as Fig.1. It is designed by the Aerodynamic Concept Design Institute of Northwestern Polytechnical University (NWPU) located in Xi'an, China. The pylon is deleted from the model to make clear the problem is only the Nacelle's position effect. The N-S equations[3] are used as the governing equations to solve the BWB's flow field. The Finite Volume method is used to discrete the equations, and the spatial discretization using the Roe's scheme. The turbulence flow model is Menter's k- ω sst model. The mesh is an O-H multi-block structure mesh as shown in Fig.2. And the calculate condition is Mach=0.8, Re=145 \times 10⁶, AOA=2°. The nacelle's position changed way is shown in Table. 1. Table. 1

Direction	Lower Bound(mm)	Upper Bound(mm)	Interval(mm)
X	-600	600	100
Y	-500	500	100
Z	-300	300	100

Some results are shown in Figures below. It could be seen from the results that there are three main effects of nacelle's position on aerodynamics of BWB: 1. The high pressure area caused by nacelle's leading edge stagnation point; 2. The shockwave interface between nacelle and wing-body; 3. The flow separation induced by the shock between nacelle and wing-body; Reference [1] R. Liebeck, M. Page, B. Rawdon. Blended-Wing-Body subsonic commercial transport[R]. AIAA 98-0438, 1998. [2] G. Hill, R. Thomas, Challenges and opportunities for noise reduction through advanced aircraft propulsion airframe integration and configurations, in: 8th CEAS Workshop: Aeroacoustics of New Aircraft and Engine Configurations, Budapest, Hungary, 2004, pp.1–13. [3] John D. Anderson, Computational Fluid Dynamics, Tsinghua University Press.

An I-integral Method for Crack Analysis in Ferroelectrics under Large-scale Switching

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ABSTRACT

It is a great challenge to extract the crack-tip fracture parameters of ferroelectrics under large-scale domain switching. A successful attempt is the establishment of the interaction integral (I-integral), whereas hereby the integration region must exclude grain boundaries. This paper breaks this limitation and develops an enhanced I-integral. The enhanced I-integral exhibits several merits over previous switching-toughening models in determining the crack-tip intensity factors. First, restriction to small-scale switching is overcome. Second, the intensity factors of different modes are decoupled. Third, it is independent of integration area size, regardless of the presence of grain boundaries and domain walls. These advantages ensure the successful utility of the area-independent I-integral in ferroelectric polycrystals under large-scale domain switching. The phase field model is combined with the I-integral method to form an effective approach to predict the polarization distributions and to evaluate the crack-tip intensity factor. Using this approach, a tensile test of PbTiO₃ ferroelectric polycrystals with an impermeable crack is simulated. The crack-tip mechanical and electrical field intensity factors obtained by the I-integral agree well with those by the extrapolation technique, and the I-integral shows good area-independence even when grain boundaries and domain walls exist in the integration area. For polycrystals, domain switching initiates not only from the crack tip but also from the grain boundaries due to high polarization gradient and stress concentration. Domain switching is triggered by a critical load, which greatly reduces the mode-I stress intensity factors. The critical load is much lower for polycrystals than for single crystals and sometimes vanishes due to grain orientations.

Direct Numerical Simulation of Thermal Turbulence and Conjugated Heat Transfer in Film-cooling Structures

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ABSTRACT

Direct Numerical Simulation of Thermal Turbulence and Conjugated Heat Transfer in Film-cooling Structures
Abstract - Nowadays, the film-cooling technology was widely applied in the design of the heated components in aero-engines, including the combustor and the turbine blades. The early researches within the field included both experimental and numerical simulation works, such as Pedersen et al[1] and Walters et al[2]. The current paper focused on the film-cooling flows in a typical simplify cylindrical-hole structure. The state-of-the-art direct numerical simulation (DNS) was used to capture the turbulent flow and the heat-transfer phenomena in the structures. In order to accurately simulate the heat-transfer in the thermal flows on both heating and cooling sides, and to strongly couple the heat-conduction calculation in the metal in between the flows, the interfacial thermal boundary conditions between the fluid and solid were implemented by the continuous conditions of both temperature and heat conduction on the heating and cooling surfaces. This simulation strategy permitted an accurate capture of the conjugated heat-transfer process in both thermal fluids and solid metal. The accurate DNS-solution techniques were achieved by the reliable and robust Flexible-cycle Additive-correction Multi-grid (FC-AC MG) method first introduced in Xu[3]. The computation provided the detailed mechanisms of the cooling-film flow formation and the closely-related thermal effects on the cooling surfaces. These results permitted an in-depth investigations of the cooling structure performance, such as the distributions of the cooling effectiveness, the flow and temperature details inside the cooling hole as well as the transient heat-conduction process inside the metal, which will eventually lead to significant improvements for the design of the current film-cooling structures. References [1]Pedersen D R, Eckertl E R G, Filming cooling with large density differences between the main stream and secondary fluid measured by heat-mass transfer analogy [J], ASME Journal of Heat Transfer, 1997, 19(1):59-98. [2]Walters D K, Lylek J H, A detailed analysis of film cooling physics, part1-streamwise injection with cylindrical holes [J], ASME Journal of Turbo Machinery, 1996, 31(3):195-216. [3]Lakehal D, Theodoridis G, Rodi W, Three dimensional flow and heat transfer calculations of film cooling at the leading edge of a symmetrical turbine blade model [J], Int. Journal of Heat & Fluid Flow, 2001, 22(2):156-160

Numerical Study on Longitudinal Vibration of Roller Chain Drive

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ABSTRACT

A refined dynamic model of a roller chain drive is developed and applied to the analysis of dynamic behavior of roller chain drive in Escalator. The roller chain drive model is composed of the two sprockets, the chain made of rollers and links, which are represented by elastic boundary constraint, lumped mass and springs-damper assemblies respectively. The chain elasticity, the mass of slack spans, torsional stiffness and inertia of sprockets are taken into account in the dynamic model. The boundary condition of the chain model are discussed in detail. The dynamic model is implemented in a computational code based on APDL to study the dynamics of the chain drive, including the frequency of longitudinal vibration and the transient vibration response of the engaging rollers under the polygonal effect. The numerical model is updated according to comparison with experiment results. Finally the updated numerical model is used to predict dynamic performance of similar roller chain drives and investigate the impacts of different factors, like length of span and mass of chain, on the dynamic behavior.

A Discrete Fiber Network Model of Arterial Elastin

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ABSTRACT

Abstract Discrete fiber network (DFN) model has been used to study biological fibrous materials with fiber-level geometric realism. DFN model is able to capture the microstructural kinematics of fibrous tissue at large strains. In most DFN models, the crosslinks were usually modeled as pin joints [1]. In this study, a DFN model of elastin network in the arterial wall was developed based on measured geometric features to study the nature of crosslinks in contributing to extracellular matrix (ECM) mechanics and fiber kinematics. Multiphoton microscopy was performed on purified elastin network from porcine thoracic aorta to characterize fiber orientation distribution, areal fraction, and fiber diameter. A DFN model was generated by randomly placing line segments into the given domain following the obtained orientation distribution until the desired fiber areal fraction was reached. The intersections of two segments were treated as crosslinks. Periodic boundary conditions were prescribed, and the DFN network is continuous when tiled up in both horizontal and vertical directions. Dangling ends, which are the free ends of line segments projecting beyond the crosslinks, were removed since they do not contribute to the rigidity of the network. Finite element simulations of DFN under equi- and nonequi- biaxial stretch were performed in Abaqus. Timoshenko beam element B21H was selected to represent a single fiber. The elastin fiber is modeled using an entropy-based freely-jointed chain with material parameters determined based on tissue-level stress vs. stretch relationship obtained from biaxial tensile tests [2]. The inter-fiber crosslinks were modeled with rotational stiffness that varies systematically from 0 (pin-joined) to infinity (rigid). The reorientation of the fibers in the DFN model was studied and compared with MPM images of elastin network. The DFN model showed excellent fitting and predicting capabilities of elastin network under equi- and nonequi-biaxial loading conditions. In previous structural based constitutive models of arteries, interactions among ECM fibers are often ignored [3]. The rotational stiffness of the crosslinks was found to play an important role in fiber realignment when elastin network is subjected to mechanical loading. References 1. Mauri, A., et al., (2016). *J Mech Behav of Biomed Mater*, 58, 45–56. 2. Wang, Y., et al., (2016). *J Biomech*, 49(12), 2358-2365.. 3. Chow, M. J., et al., (2014). *Biophys. J*, 106(12), 2684–2692.

Error Estimates for Dynamic Augmented Lagrangian Boundary Condition Enforcement, with Application to Immersogeometric Fluid--Structure Interaction

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ABSTRACT

In this work, we analyze the convergence of the recent numerical method for enforcing fluid--structure interaction (FSI) kinematic constraints in the immersogeometric framework for cardiovascular fluid--structure interaction. In the immersogeometric framework, the structure is modeled as a thin shell, and its influence on the fluid subproblem is imposed as a forcing term. This force has the interpretation of a Lagrange multiplier field supplemented by penalty forces, in an augmented Lagrangian formulation of the FSI kinematic constraints. Because of the non-matching fluid and structure discretizations used, no discrete inf-sup condition can be assumed. To avoid solving (potentially unstable) discrete saddle point problems, the penalty forces are treated implicitly and the multiplier field is updated explicitly. In the present contribution, we introduce the term dynamic augmented Lagrangian (DAL) to describe this time integration scheme. We formulate the DAL algorithm for a linearized parabolic model problem, analyze the regularity of solutions to this problem, and provide error estimates for the DAL method in both the $L^\infty(H^1)$ and $L^\infty(L^2)$ norms. We also prove error estimates for a recently-proposed extension of the DAL method, with improved conservation properties. Numerical experiments indicate that the derived estimates are sharp and that the results of the model problem analysis can be extrapolated to the setting of nonlinear FSI, for which the numerical method was originally proposed.

Interfacial Behavior of Adhesively Bonded Pipe Joints Subjected to Combined Thermal and Mechanical Loadings

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ABSTRACT

Pipe structures are a very important structural form for energy, aerospace and construction industries. In consideration of whole weight, strength and maintenance workload, it is commonly accepted that there should be less joints in a piping system at first design. Due to the limitation of transportation, installation and rehabilitation, a joint seems essential for a large structure system containing different components. The limitations of the overall system performance usually come from the capacity of pipe joints. For most piping system, the joints can be divided into three types: flange coupling, welding and adhesive bonding. The first two traditional connections have the same shortage, such as high stress concentration. However, the adhesively bonded pipe joint can effectively lower the stress concentration. Among all the possible loading configurations, tensional loading is one of the fundamental loading types. Because of the difficulties in the analysis of interfacial behavior, there are just a few theoretical studies available in the previous references. All the existing analytical studies were focused on the elastic region of interfacial behavior. However, the interfacial failure always experiences much more complicated processes. So the softening and debonding of the adhesively bonded interface should be taken into consideration. To understand the interfacial behavior of plane joints exposed to different temperature variations, the pull test can be used. The results can reflect the combined effects of a number of factors, including temperature-induced interfacial shear stresses change in the bondline as well as the adherends if the temperature becomes sufficiently high. The whole joints should be subjected to normal work high temperature because a large temperature variation will induce complicity of the interface bond property. Interfacial behavior is the key factor that affects the total performance of bonded joints. This paper presents an analytical solution for the full-range behavior of an adhesively bonded pipe joint under combined thermal and mechanical loadings in which interfacial softening and debonding have been taken into consideration. The expressions for the interface slip and shear stress are derived for the different failure stages. The present research improves and clarifies the understanding of the interfacial debonding of bonded pipe joints under combined thermal and mechanical loadings. The predictions of the closed-form solutions agree with the ABAQUS finite element results very well. By modifying different material parameters, the present results may be further extended to composite pipe joints, composite-metal pipe joints or metallic pipe joints.

Computational Mechanics Modeling of a Continuum Soft Robot

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ABSTRACT

Compliant and low-weight soft robots have many advantages, compared to traditional rigid robots, including safe operation in constrained environments, dexterity and adaptivity in unstructured environments, relative simplicity in fabrication, low-energy consumption, and low-cost. One of many challenges in developing soft robots is the mechanics modeling and control of soft robots due to continuum elastic deformation of the soft materials. In this work, we develop a computational mechanics program for simulation and control of a novel cable-driven continuum soft robot. A 3D finite-element rod model is adopted to convert the continuum robot arm into discrete rigid bodies in the computational program. Computational multibody dynamics algorithms are adopted to carry out dynamic simulations of the robot arm driven by the motor-cable forces. The friction and contact of robot arm with the environment are simulated. The computational mechanics program is used to guide and optimize the design of the continuum soft robots for specific tasks such as locomotion. Simulations from the computational program are also used in a machine-learning algorithm to develop an adaptive control method for the soft robots.

A Modified Zerilli–Armstrong Model Incorporating the Anisotropy and Anomalous Stress Peak : Application to the Laser Additive Manufactured Inconel 718

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ABSTRACT

Abstract: The lack of accurate description of dynamic thermomechanical behaviors in extreme high-strain-rate and high-temperature loading environment could be a major obstacle to extending the laser additive manufactured (LAMED) Inconel 718 to engineering applications. In this study, to obtain further understandings of plastic flow behaviour of the LAMED Inconel 718, uniaxial compression experiments were conducted over a wide range of temperatures (298–1193 K) and strain rates (0.001–5300/s). Not only the anisotropy of compressive strength, but the influences of temperature and strain rate on plastic flow stress were analyzed. The flow stress of the as-deposited alloy in laser scanning direction is higher than that in deposition direction, which is attributed to the columnar crystal epitaxially growing along the build direction. A anomalous stress peak in flow stress vs. temperature relation was found and proved to be the third-type of strain aging effect. The flow stress of the alloy exhibits inconspicuous strain-rate sensitivity over the range of strain rate below 1000 /s, while increases sharply with the strain rate once it exceeds 1000 /s. Taking into account the anisotropy, as well as the anomalous temperature and strain rate dependencies of the flow stress, a modified Zerilli–Armstrong constitutive model for the LAMED In718 was developed. A directional factor was introduced to indicate the equivalent size of columnar crystals, the strain rate hardening has been enhanced once the strain rate exceeds a certain level, and a normal distribution with temperature was used to describe the 3rd SA effect. The model was shown to be able to accurately predict the plastic flow behaviour of the LAMED Inconel 718 over a wide range of temperatures and strain rates.

Keywords: Laser additive manufactured Inconel 718, anisotropy, temperature, strain rate, constitutive model

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A Parallel Adaptive Mesh Flow Solver Based on PHG Toolbox

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ABSTRACT

Nowadays unstructured tetrahedral grids are widely used in scientific and engineering computing. Adaptive mesh strategies can improve accuracy for a given number of grid scales, or reduce grid scales for a given accuracy. In the past two decades a lot of parallel unstructured flow solvers have been developed. However, development of parallel adaptive mesh codes needs a series of efforts ranging from domain repartition to keep load balance to data transfer among processors, which are barriers for many people only caring numerical schemes or engineering applications. The emergence of a PHG (Parallel Hierarchical Grid) platform provides interface functions for carrying out common and difficult tasks in parallel adaptive finite element programs, such as parallel adaptive mesh refinement, dynamic load balancing, and linear solvers. PHG is an open source toolbox for writing scalable parallel adaptive finite element programs. In this work, we have developed a C++ h-adaptive code – Libfvphg for numerical solution of hyperbolic conservation laws / Euler equations on three-dimensional tetrahedral grids based on the PHG platform. Libfvphg uses finite volume method with linear reconstructions but it is easily extendable to discontinuous Galerkin methods directly. This is because PHG supports DG finite element as well as other types of element. The finite volume method uses only the piecewise constant element. Libfvphg not only encompasses a variant of partial differential equations (conservation laws, Euler), reconstruction strategies (Green Gauss, least squares) and numerical flux functions (LF, HLLC, Roe), but also supports various posteriori error estimates for adaptive mesh. We show that the development of Libfvphg using PHG is like writing a serial code, where the DOF of PHG is used as the flow variables. The needed neighboring cell information in other process and parallel adaptive mesh management are automatically done in PHG. We describe the C++ object hierarchy, the sets of equations used in the current version, and the available choices for numerical discretization, particularly, the second-order high resolution multidimensional limiting process (MLP). Finally, we give a set of relevant validation and verification test cases. These include spherical explosion, transonic flow past a wing-body combination. Numerical effects of using different reconstructions and posteriori error estimates are examined. The parallel efficiency is shown to be 80-40% from 32 up to 1024 processes for 20 million tetrahedrons. We intend to illustrate that parallel unstructured grid flow solver can be built relatively easy if using the PHG platform.

N-Scale Eigenstrain-Based Reduced Order Homogenization

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ABSTRACT

A hierarchical model reduction approach aimed at systematically reducing computational complexity of multiple scale homogenization for nonlinear history-dependent problems is developed. The method consists of the following salient features: (1) formulation of non-linear unit cell problems at multiple scales in terms of eigenstrain modes that a priori satisfy equilibrium equations at multiple scales and thus eliminating the need for costly solution of discretized non-linear equilibrium, (2) hierarchical solution strategy that requires sequential solution of single-scale problems, and (3) recursive formulation of N-scale stress updates that essentially simplifies the implementation to a regular two-scale case.

A Generalized Dual-Purposed Reduced-Order-Homogenization Model for Multiscale Fatigue Damage

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ABSTRACT

Composite material is widely used as a thin-wall structure, where the characteristic length in thickness direction (out-of-plane direction) is much smaller than the rest two directions (in-plane direction). In addition, the composite structure is made of a number of layups with different orientations. Accordingly, delamination may take place between layups where the mismatch stress reaches the corresponding strength. In the presentation, we describe a Generalized Dual-Purpose Model (GDPM). The GDPM is able to predict interlayer delamination under mode I, II, III, or generalized mixed-mode, where the intralayer can be arbitrary plane-stress model. Specifically, the intralayer adopts a plane stress multiscale reduced-order-homogenization model to simulate fatigue damage accumulation of a Polymer Matrix Composite (PMC) material. An isotropic fatigue damage model and hybrid fatigue damage and plasticity model are introduced to simulate the fiber and matrix phase, respectively. Comparison of the numerical results with experimental measurement is given as well.

Experimental and Numerical Investigations of 6082-T6 Aluminum Alloy Beams with Hollow Sections

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ABSTRACT

This paper presents experimental and numerical studies of aluminum alloy beams with square (SHS), rectangular (RHS) and circular (CHS) hollow sections. Three-point bending and four-point bending tests were performed to the hinged-ended beams made of cold-extruded 6082-T6 aluminum alloy and measurement of the initial geometric imperfection and material strength for the members was conducted before the tests. A finite element (FE) model was proposed using non-linear FE analysis software ABAQUS and the model was verified against the experimental results. Considering the distinct nonlinear property of aluminum alloy, material and geometric nonlinearities were incorporated into the FE model. The simulation results showed that the FE model was accurate enough to predict the failure modes, buckling resistance and deformability of the experimental beams. A parametric study was conducted to access the effect of the key parameters such as sectional dimension, radius-thickness ratio and slenderness ratio on the deformation capacity and strength of the hinged-ended aluminum alloy beams by the FE model. Based on the comparison of the beam strengths obtained from the parametric study and the design strength predicted by several current design specifications, the verification of the Chinese code (GB 50429-2007), the American code (ADM-2005) and the European code (Eurocode 9) were performed and the revised suggestions for GB 50429-2007 were presented. The reliability analysis for the design rules were performed to investigate whether the reliability levels can reach the goals.

CFD Based Multidisciplinary Design Optimization for Offshore Aquaculture Platform

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ABSTRACT

The shape of the hull has a significant impact on the resistance and propulsive performance of the ship, especially for the fat ship. In this research, the experimental and numerical analysis of an offshore aquaculture platform are carried out, while the multidisciplinary design optimization of the platform shape is also conducted. RANS solver is applied for the numerical analysis. Validity of the numerical method is proved by comparing numerical results of the original shape with experimental results. An optimization framework using Latin hypercube design, free-form deformation (FFD) method, Kriging surrogate model and Genetic algorithm (GA) are developed. Nine design variables have been employed to modify the shape of the platform. Because of a tradeoff between the minimum resistance and the minimum nonuniformity of wake flow, the optimum solution of the hull shape is selected from the Pareto front to balance the two objectives. Model tests for the optimized shape are then performed to validate the design results. The results show that the resistance and the nonuniformity of the wake flow of the optimized shape are reduced by 1.59% and 17.80% respectively in comparison with the results of the original shape.

A Probabilistic Progressive Damage Simulation Model for Braided Composites

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ABSTRACT

A Probabilistic Progressive Damage Simulation Model for Braided Composites Sungwoo Jeong Department of Mechanical & Aerospace Engineering, Seoul National University, South Korea Chao Zhang School of Aeronautics, Northwestern Polytechnical University, China Gunjin Yun Department of Mechanical & Aerospace Engineering, Seoul National University, South Korea Abstract This paper presents a probabilistic progressive damage simulation model for braided composites. Damage mechanisms considered in this paper are fiber tow damage and tow-to-tow interface delamination. Deterministic predictions by the existing damage progressive analysis model of braided composites could be very different from the experimental global strength and failure modes due to effects of material uncertainties. Therefore, uncertainties of constituents' physical properties were taken into account in this study. An anisotropic damage model was used for damage initiation and evolution of fiber tows. A cohesive-zone model under mixed-modes was also adopted for delamination between fiber bundles. Strength and critical fracture energies of fiber tows were simulated as spatially varying random fields through the Karhunen-Loeve expansion method. For demonstrations of the proposed probabilistic damage analysis, a three-dimensional meso-scale finite element model of a single-layered unit cell was developed. Sensitivity of statistical parameters of the random material properties to sequential local and global damage behavior was evaluated. Both statistical local damage and global response of the braided composite were simulated and compared with experimental observations and we identified the most sensitive statistical model parameters. Keywords: spatial variability, probabilistic damage progression, braided composites, random fields, stochastic analysis, Karhunen-Loeve expansion

Large-scale Thermal Elastic-Plastic Welding Analysis Using Domain Decomposition Method

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ABSTRACT

To estimate mechanical behaviors of a welding problem, such as residual stress and residual deformation, thermal elastic-plastic analysis is helpful. Also, when the problem is a real structure, large-scale parallel computation technique is necessary. Thus, we are developing a system that can analyze a large-scale welding problem by thermal elastic-plastic modeling. This system is based on domain decomposition method, which is frequently used in parallel finite element analysis. In domain decomposition method, the analysis domain is decomposed into multiple subdomains. Then, a linear system of equations, which is linearized by Newton-Raphson method, is statically condensed into subdomain interface degrees of freedom. The condensed linear system of equations is solved by conjugate gradient method with a preconditioner such as balancing domain decomposition. In the presentation, we will show the methodology that is specially required in the large-scale welding analysis. For example, the consideration of a moving heat source needs MPI (message passing interface) communications at every time step. Moreover, the convergence properties of Newton-Raphson method as well as conjugate gradient method are carefully investigated. This is because the thermal elastic-plastic problem with temperature-dependent material parameters is known to be a strongly nonlinear problem especially in the vicinity of the heat source. A part of the present work has been supported by JSPS KAKENHI Grant Number JP16K05988.

Sharp Volumetric Billboard Based Multilevel Modeling and Multigrid Method

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ABSTRACT

Numerical modeling of heterogeneous materials is challenging due to the extremely high computational cost required to resolve all of the geometrical complexities. Despite the recent development of high performance computational frameworks and homogenization techniques, accurately predicting highly nonlinear material response with prominent localized behavior remains elusive. In this talk, we will introduce a novo sharp volumetric billboard (SVB) based multilevel modeling and multigrid computational technique, which enables accurate predictions of mechanical behavior of high energy ball milled (HEBM) Ni/Al composites. This SVB based modeling is an image based modeling technique, which stems from the volumetric billboard (VB) method, a Google Earth like multi-resolution modeling strategy in computer graphics. 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 the Ni/Al reactive composites produced by HEBM. 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. Then, we use a parallel generalized finite element code, PGFem3D, to compute the mechanical behavior under a tension-relaxation loading profile using crystal plasticity constitutive equations. We adopt both identical and random texture. The macro- and micro-mechanical robustness of data compression is demonstrated through corresponding error analysis. The close properties of SVB LODs and their data structures naturally lend themselves in the development of multigrid methods. Our recent study shows that the SVB LODs contains reliable coarse microstructures, which can instruct the formulation of the key component – the intergrid operators -- in a multigrid method. Moreover, the coarse SVB LODs can also act as reliable preliminary to large computations. This is because the coarse SVB LODs generate coarse problems that can be used to approximate finer solution using significantly lower computational resources with acceptable numerical error.

Investigating the Influence of Buccal Bone Thickness on Bone Remodeling around Maxillary Anterior Implantation

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ABSTRACT

Due to the anatomical registration in the maxillary anterior region during implantation, such as insufficient bone volume, part of the buccal bone will be lost after bone remodeling, with the consequence of a high risk of soft tissue recession [1]. Therefore, the critical buccal bone morphology around implants is widely considered as a primary factor to decelerate bone resorption around implants [2], as increasing the buccal bone thickness (BBT) above the implant [3]. This study established a framework that combined the in-vivo clinical quantification with in-silico computational modeling to investigate the effects of BBT on the bone remodeling outcome. One specific patient who had undergone an implant treatment in the anterior maxilla and experienced the buccal bone resorption on the implant was studied. A three-dimensional heterogeneous nonlinear FE model was constructed based on the CT images of this patient, and a validated bone remodeling algorithm was employed to simulate up to 48-month bone remodeling behavior in the bone region around the implant. The anterior incisory bone region of this model was then varied systematically to simulate five different BBTs (0.5, 1.0, 1.5, 2.0, and 2.5 mm), and the optimal BBT was inversely determined to minimize the risk of resorption. Our findings indicated that the initial BBT appeared to play a critical role in distributing mechanobiological stimuli, thereby determining subsequent variation in BBT. For this particular patient, the simulated results revealed that the increased BBT decreases the bone resorption rate in the peri-implant region. However, a 1.5 mm of BBT is recommended in this case as the extra bone volume does not indicate improving the remodeling outcome. This study revealed that the initial BBT significantly affected mechanobiological responses, which consequentially determines the bone remodeling process. An optimal initial BBT is considered essential to assure a long-term stability of implant treatment. Reference 1. Grunder U, et al. 2005. Influence of the 3-d bone-to-implant relationship on esthetics. *Int J Periodontics Restorative Dent*. 2. Merheb J, et al. 2014. Critical buccal bone dimensions along implants. *Periodontology* 3. Veltri M, et al. 2015. Three-dimensional buccal bone anatomy and aesthetic outcome of single dental implants replacing maxillary incisors. *Clinical oral implants research*.

Bayesian Deep Convolutional Encoder-Decoder Networks for Surrogate Modeling and Uncertainty Quantification

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ABSTRACT

We are interested in the development of surrogate models for uncertainty quantification and propagation in problems governed by stochastic PDEs using a deep convolutional encoder-decoder network in a similar fashion to approaches used in deep learning for image to image regression tasks. To evaluate the performance of this approach, we consider standard uncertainty quantification benchmark problems including flow in heterogeneous media defined in terms of limited data-driven permeability realizations. The performance of the surrogate model developed is surprisingly good even though there is no underlying structure shared between the input (permeability) and output (flow/pressure) fields as is often the case in the image-to-image regression models used in computer vision problems. Since normal neural networks are data intensive and cannot provide predictive uncertainty, we propose a Bayesian approach to convolutional neural nets. A recently introduced variational gradient descent algorithm based on Stein's method is scaled to deep convolutional networks to perform approximate Bayesian inference on millions of uncertain network parameters. This approach achieves state of the art performance in terms of predictive accuracy and uncertainty quantification in comparison to other approaches in Bayesian neural networks as well as techniques such as Gaussian processes and ensemble methods even when the training data size is relatively small. Uncertainty propagation tasks are considered and the predictive output Bayesian statistics are compared to those obtained with Monte Carlo estimates.

Computational Homogenization of MREs: Effect of Boundary Conditions, RVE Size and Microstructure Composition

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ABSTRACT

Magnetorheological elastomers (MREs) are composites whose mechanical behaviour highly depends on the applied magnetic field. Since explicit constitutive laws for such heterogeneous materials are not specified, their effective macroscopic properties can be estimated from the response of the underlying micro-structures using homogenization procedure. In the present work, the behaviour of heterogeneous magnetorheological composites subjected to large deformations and external magnetic fields is studied. A fully-coupled FE² computational homogenization framework is used to derive the macroscopic material response from the averaged responses of the underlying periodic and random microstructures. The microstructures consist of two materials and are far smaller than the characteristic length of the macroscopic problem. Different types of boundary conditions based on the primary variables of the magneto-elastic enthalpy and energy functionals are applied to solve the problem at the micro-scale. The results indicate that the application of each set of boundary conditions presents a different macroscopic responses. However, increasing the size of the RVE, solutions from different boundary conditions and microstructures converge to the response obtained from periodic boundary conditions.

Why Aortic Valve Functions The Way It Does

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ABSTRACT

Understanding the mechanics of the aortic valve (AV) has been a research focus for many years, with the aim of improving our understanding of its function in health and disease, as well as guiding the design of prosthetic replacements. Yet, we still do not fully understand how the AV is “designed,” including what features are most critical to ensure its efficient operation during the cardiac cycle. In the present study, we utilized a computational framework to determine how key characteristics of the AV interact and vary, while still maintaining proper valve function. Major AV features simulated included leaflet geometry and anatomical asymmetry, heterogeneity, prestrain, anisotropy, and layer contributions, as well as the shape and mechanical behaviors of the aortic sinus and aortic walls. AV dynamics and performance were assessed by a number of metrics, including effective orifice area, wall shear stresses, and leaflet coaptation, stress and strain fields within the leaflets and aortic root. To achieve this computationally, we simulated the coupling of the deforming aortic root, heart valves, and the surrounding blood flow under physiological conditions through several cardiac cycles using our immersogeometric fluid-structure interaction (FSI) methodology. Leaflets were modeled as a thin shell structures using various material behaviors and structural features. In particular, effects of leaflet shape, heterogenous structure, and interactions with the aortic root and sinus were studied in detail. We observed a noticeable influence of the surface curvature on the effective orifice area of the valve and the overall leaflet deformation. Sensitivity results also demonstrated that incorporating an anisotropic material model for leaflets had a significant influence on the valve deformation during diastolic closure. The basis for this was noted in part that in dynamic simulation of the AV during the opening phase the leaflet was in the small strain regime, when the majority of the collagen fibers were not recruited, so that the isotropic like tissue matrix dominated the valve deformation. Geometric studies clearly delineated the range of leaflet shapes acceptable for physiological function, and in particular what characteristics might be allowable in prosthetic valve devices. The results of this study demonstrate the effectiveness of the proposed platform for analyzing the heart valve function with greater levels of physical realism, and can provide guidelines for detecting anomalies in the natural valve or improving leaflet tissue’s design in the artificial valves to enhance valve durability.

Numerical Simulation of Free Fall Penetrometer Deployment Using MPM

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ABSTRACT

The number of engineering activities in offshore and nearshore environments is increasing because of the growing population in coastal areas, the necessity to obtain energy and minerals from the seafloor, and the current advances in ocean and offshore energy harvesting. In-situ characterization of seabed sediments is essential to most of such projects. However, current standard methods such as Cone Penetration Testing is expensive, time-consuming, and challenged by environmental conditions. Free fall penetrometers (FFP) promise the characterization of surficial seabed sediments efficiently and can be adapted to different environmental conditions. FFPs can be described as torpedo-like bodies equipped with various sensors. Recently, focus was given to devices that only measure accelerations and pore pressure in the interest to design more robust devices. The penetrometer free falls through the water column and impacts the surface at 3-6 m/s. The reaction force on the tip is computed using acceleration recordings, and sediment strength properties are deduced. However, soil behavior during high and transient velocities impacts is not fully understood, yet. Hence, there is a need to perform numerical simulations to investigate the problem. Modelling of a FFP deployment is complex because represents a soil-structure interaction problem involving high-velocity motions, large deformations, and hydro-mechanical coupling between soil particles and porous water. Several numerical technics have been previously used, including Finite Element Method (FEM), Arbitrary Lagrangian-Eulerian Method (ALE), and Coupled Eulerian-Lagrangian method (CEL). However, FEM is limited to small deformations, while ALE and CEL require remeshing techniques to deal with large strains. In this study, the Material Point Method (MPM) is proposed to analyze the FFP performance. MPM can accommodate large deformations without mesh tangling limitations, contact between soil and structure can be easily simulated, and coupled hydro-mechanical formulations can be considered. A set of numerical analysis will be performed to determine the capabilities of MPM to model FFP deployments. A moving mesh technique will be considered together with a mesh convergence analyses to optimize the computational resources and to maximize the results accuracy. The interaction between penetrometer and soil will be simulated considering different contact properties using a contact algorithm. A hydro-mechanical formulation will be considered to simulate the behavior of saturated soil. The numerical results will be compared and benchmarked with experimental data. Finally, a parametric study will be conducted to investigate the relationships between dynamic bearing capacity, FFP velocity, and soil strength properties.

Mean Field Theory of Plasticity and Yielding of Glasses

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ABSTRACT

I will discuss a microscopic mean field theory of glasses. The theory is based on an exact solution of interacting particle systems in the abstract limit of infinite dimensions. Within the theory, one can follow the response of a glass state to several perturbations, including compression and shear. I will focus in particular on the response to shear, and discuss how the theory can reproduce some known features of glasses, such as plasticity and yielding. I will also discuss the limitations of the theory, and how to go beyond mean field. The talk is based on [1] Shear yielding and shear jamming of dense hard sphere glasses - P.Urbani, F.Zamponi - Phys.Rev.Lett. 118, 038001 (2017) [2] Following the Evolution of Hard Sphere Glasses in Infinite Dimensions under External Perturbations: Compression and Shear Strain - C.Rainone, P.Urbani, H.Yoshino, F.Zamponi - Phys.Rev.Lett. 114, 015701 (2015)

A COMPUTATIONAL APPROACH FOR INVESTIGATION OF THE EFFECT OF ELECTROMAGNETIC PHENOMENA IN MAGNETORHEOLOGICAL SQUEEZE FILM DAMPERS ON THE VIBRATION ATTENUATION OF RIGID ROTORS

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Key words: magnetorheological squeeze film dampers, variable magnetic reluctance, transient electromagnetic phenomena, current and voltage control, rotor vibration attenuation

Abstract. The optimum performance of damping devices placed between the rotor and its stationary part is achieved by adapting their damping effect to the current running conditions. This is enabled by application of magnetorheological squeeze film dampers, the damping force magnitude of which is controlled by changing magnetic flux passing through a thin layer of lubricating film. The magnetic flux is generated in electric coils embedded in the damper body. The change of the thickness of the oil film around the damper circumference due to the rotor vibration changes reluctance of the magnetic circuit. It induces the electromotoric voltage that reduces the applied current and thus leads to decreasing of amount of the damping effect. In the developed mathematical model of the damper the magnetorheological oil was represented by a bilinear material. The dependence of the yielding shear stress on magnetic induction was described by a power function, the pressure distribution in the oil film by the modified Reynolds equation, and the electromagnetic phenomena by the equation of the voltage equilibrium and the Hopkins law. The developed mathematical model was used to compare the influence of two strategies for controlling the damping effect, the current and voltage control, on vibration suppression of rotor systems. The development of the enhanced mathematical model of the magnetorheological squeeze

film damper and learning more on the influence of the control regimes on behaviour of rigid rotors are the main contributions of this paper.

1 INTRODUCTION

The lateral vibration of rotating machines is attenuated by damping devices inserted in the rotor supports. As discussed in [1] to achieve their optimum performance their damping effect must be adaptable to the current operating speed.

The work of controllable damping devices is based on utilization of various physical principles, like hydraulic [2], mechanical-hydraulic [3] or electromagnetic [4].

A new approach to controlling the damping forces is utilized in the magnetorheological dampers, which are lubricated by liquids sensitive to a magnetic field. The damping force is controlled by a magnetic flux passing through the lubrication layer. The design, function, experimental investigations and application of magnetorheological dampers for the vibration attenuation of rotating machines are discussed in a number of journal articles and conference papers, e.g. in [5,6]. Zapoměl et al. [7] developed the mathematical model of a short squeeze film magnetorheological damper, in which bilinear material was employed to represent the magnetorheological oil. This arrived at stable computational procedures, in which this damper model was implemented. The study reported in [8] deals with the distribution of the magnetic flux in the damper body and of the magnetic induction in the lubricating film.

This article extends the mathematical model of a magnetorheological squeeze film damper by taking into account variable reluctance of the magnetic circuit and deals with the influence of the induced electromagnetic phenomena during the damper operation on the time delay of the damping effect and consequently, on vibration attenuation of rigid rotors. The developed mathematical model was used to compare the influence of two strategies for controlling the damping force, the current and voltage control, focusing on the vibration suppression of rotor systems.

2 MECHANICAL AND HYDRAULIC MODEL OF THE DAMPER

The principle of work of magnetorheological squeeze film dampers (Fig. 1) is described in detail in [7,9]. The damping effect is produced by squeezing a thin layer of a magnetorheological oil between two concentric rings. The inner ring is connected with the shaft journal by a rolling element bearing and with the damper housing by a flexible cage spring. The magnetic flux generated in electric coils embedded in the damper passes through the lubricant. As resistance against the flow of magnetorheological oils depends on magnetic induction, the change of the coil feeding voltage can control the amount of the damping force.

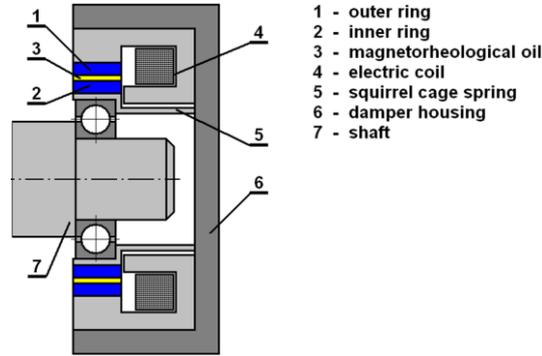


Fig. 1. Scheme of the magnetorheological squeeze film damper.

The pressure distribution in the oil film is described by the Reynolds equation adapted to bilinear material. The derivation and details on solution of the governing equations can be found in [7].

$$\frac{\partial}{\partial Z} \left(\frac{1}{\eta_c} h^3 p' \right) = 12\dot{h} \quad \text{for } 0 \leq Z \leq Z_c, \quad (1)$$

$$\frac{\partial}{\partial Z} \left[\frac{1}{\eta} \left(h^3 p' + 3h^2 \tau_y + 8 \frac{\tau_c^3}{p'^2} - 12 \frac{\tau_y \tau_c^2}{p'^2} \right) - \frac{8}{\eta_c} \frac{\tau_c^3}{p'^2} \right] = 12\dot{h} \quad \text{for } \dot{h} < 0 \quad \text{and} \quad Z > Z_c, \quad (2)$$

$$Z_c = -\frac{\tau_c h^2}{6\eta_c \dot{h}}, \quad (3)$$

$$p'_c = -\frac{2\tau_c}{h}. \quad (4)$$

Here, p is the pressure, p' stands for the pressure gradient in the axial direction, Z is the axial coordinate perpendicular to axes X and Y (Fig. 2), h is the oil film thickness, τ_y is the yielding shear stress, τ_c is the shear stress at the core border (the core is the region in the oil layer where the velocity rate is low and the oil behaves almost as a solid matter [10]), η_c , η are the dynamic viscosities of the oil inside and outside the core area, respectively, Z_c defines the axial coordinate of the location where the core touches the rings surfaces, p'_c denotes the pressure gradient in the axial direction at location Z_c , and $(\dot{})$ denotes the first derivative with respect to time.

At locations where the thickness of the oil layer rises with time ($\dot{h} > 0$), a cavitation is assumed. It is supposed that the pressure remains constant in cavitated areas and is equal to the pressure in the ambient space [11].

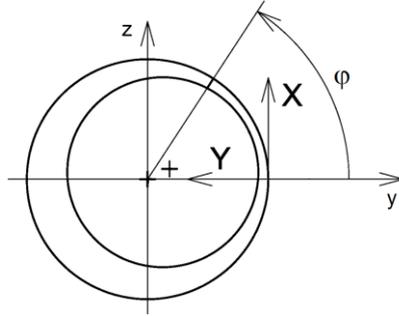


Fig. 2. The coordinate system of the damper.

The components of the hydraulic force acting on the rotor journal in the y and z directions (F_{mry} , F_{mrz}) are given by the integration of the pressure distribution p_d in the damper gap

$$F_{mry} = -2R_D \int_0^{\frac{L_D}{2}} \int_0^{2\pi} p_d \cos \varphi \, d\varphi \, dZ, \quad (5)$$

$$F_{mrz} = -2R_D \int_0^{\frac{L_D}{2}} \int_0^{2\pi} p_d \sin \varphi \, d\varphi \, dZ \quad (6)$$

taking into account different pressure profiles in noncavitated and cavitated regions. R_D is the mean gap radius, L_D is the damper length, and φ is the circumferential coordinate (Fig. 2).

3 ELECTROMAGNETIC MODEL OF THE DAMPER

The damper body is considered to be consisted of a set of meridian segments and each segment as a divided core of an electromagnet. This enables to express magnetic induction B and consequently, the yielding shear stress at any location in the oil film [7,9]

$$B = k_B \mu_0 \mu_{MR} \frac{I}{h} \quad (7)$$

$$\tau_y = k_y B^{n_y} \quad (8)$$

Here, μ_0 is the vacuum permeability, μ_{MR} is the magnetorheological oil relative permeability, I is the applied current, k_B is the design parameter, and k_y and n_y are the proportional and exponential material constants of the magnetorheological oil. More details on determination of the design parameter k_B can be found in [8].

Lateral vibration of the inner damper ring changes the width of the damper gap and thus the magnetic flux passing through the oil layer. The relation between the applied voltage, applied current and the magnetic flux is governed by the equation of the voltage equilibrium

$$\frac{d\Phi}{dt} + RI = U, \quad (9)$$

Φ is the magnetic flux generated in the coil, R is the ohmic resistivity of the electric circuit, U is the applied voltage, and t is the time.

The Hopkins law and the assumption that relative permeability of the damper steel part is much larger than that of the magnetorheological oil gives the relation for the amount of the magnetic flux passing through each meridian segment

$$N_C I = \Phi_i \frac{h_i}{\mu_{MR} R_D L_D \Delta\varphi}, \quad (10)$$

$\Delta\varphi$ is the increment of the circumferential coordinate, N_C reads for the number of the coil turns.

The total magnetic flux is equal to the sum of magnetic fluxes passing through all meridian segments

$$\Phi = \sum_{i=1}^{N_s} \Phi_i, \quad (11)$$

where N_s is the number of the meridian segments.

Next it is assumed that the segments are of an infinitesimal thickness. Then introducing

$$A = \int_0^{2\pi} \frac{d\varphi}{h(\varphi)}, \quad (12)$$

expressing Φ_i from (10) and utilization of (11) and (12) give the relation for the total magnetic flux

$$\Phi = \mu_{MR} N_C I R_D L_D A(t). \quad (13)$$

The differentiation of (13) with respect to time and its substitution into (9) yields the governing equation for the time history of the current in dependence of the applied voltage

$$\dot{I} + \left(\frac{\dot{A}}{A} + \frac{R}{\mu_{MR} N_C R_D L_D A} \right) I = \frac{U}{\mu_{MR} N_C R_D L_D A}. \quad (14)$$

4 THE INVESTIGATED ROTOR

The rotor of the analysed rotating machine consists of a shaft and of one disc (Fig. 3). The rotor is connected with the stationary part by two magnetorheological dampers at both its ends. It turns at constant angular speed, is loaded by its weight, and is excited by the disc unbalance. The cage springs of both dampers are prestressed to eliminate their deflection caused by the rotor weight. The rotor and the stationary part can be considered as absolutely rigid and the whole system as symmetric with respect to the disc middle plane.

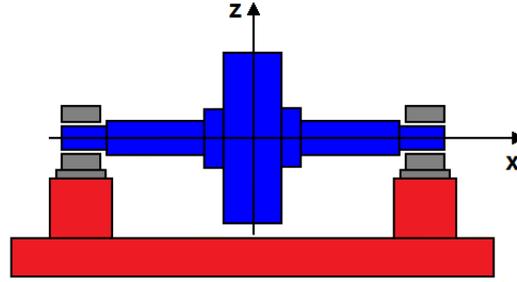


Fig. 3. The investigated rotating machine.

The task was to compare two approaches to controlling the damping force produced by the magnetorheological dampers, the current and voltage control, by analysing the rotor response on the change of the damping effect.

In the computational model the rotor is considered as absolutely rigid body and the magnetorheological dampers are represented by springs and force couplings.

The vibration of the system, taking into account its symmetry, is governed by a set of two nonlinear motion equations

$$m_R \ddot{y} + b_P \dot{y} + 2k_D y = 2F_{mry} + m_R e_T \omega^2 \cos \omega t + F_{psy}. \quad (15)$$

$$m_R \ddot{z} + b_P \dot{z} + 2k_D z = 2F_{mrz} + m_R e_T \omega^2 \sin \omega t + F_{psz} - m_R g. \quad (16)$$

m_R is the rotor mass, b_P is the coefficient of external damping, k_D is the stiffness of the cage spring, ω is the angular speed of the rotor rotation, e_T is the eccentricity of the rotor unbalance, y, z are the displacements of the rotor centre, F_{psy}, F_{psz} are the y and z components of the prestress force, g is the gravity acceleration, and $(\ddot{\cdot})$ denotes the second derivative with respect to time.

To perform the solution the equations of motion were transformed to the state space. In the case of the voltage control the equation governing the dependence of the current on the applied voltage feeding the magnetorheological dampers was added. The Adams-Moulton method was applied to solve the resulting equations.

5 THE SIMULATION RESULTS

The parameters of the studied rotor are: the rotor mass 430 kg, the coefficient of linear damping of the rotor caused by the environment 200 Ns/m, the stiffness of one cage spring 3.0 MN/m, the eccentricity of the rotor unbalance 60 μm , the magnetorheological squeeze film damper length/diameter 50/150 mm, the width of the damper gap 1.0 mm, the oil dynamic viscosity outside the core 0.3 Pas, the oil dynamic viscosity in the core 300 Pas, the magnetorheological oil proportional and exponential constants 2000, 1.1, respectively, the oil relative permeability 5, the damper design parameter 120, the resistivity of the electric circuit 10 Ω , and the number of the coil turns 240.

A simple dynamical analysis shows that the critical speed of the undamped rotating system is about 118 rad/s.

The goal of the investigation was to analyse the rotor response on increase of the damping effect for several angular velocities of the rotor rotation (100, 120, 250, 500 rad/s). They correspond to the speeds below, close to, and above the critical one. The rise of damping in the magnetorheological dampers was controlled by the uniform increase of the current (current control) or voltage (voltage control) during the time period of 10 ms. The increase was 0.5A/5V, 0.5A/5V, 2A/20V, 3A/30V for speeds of 100, 120, 250, 500 rad/s, respectively.

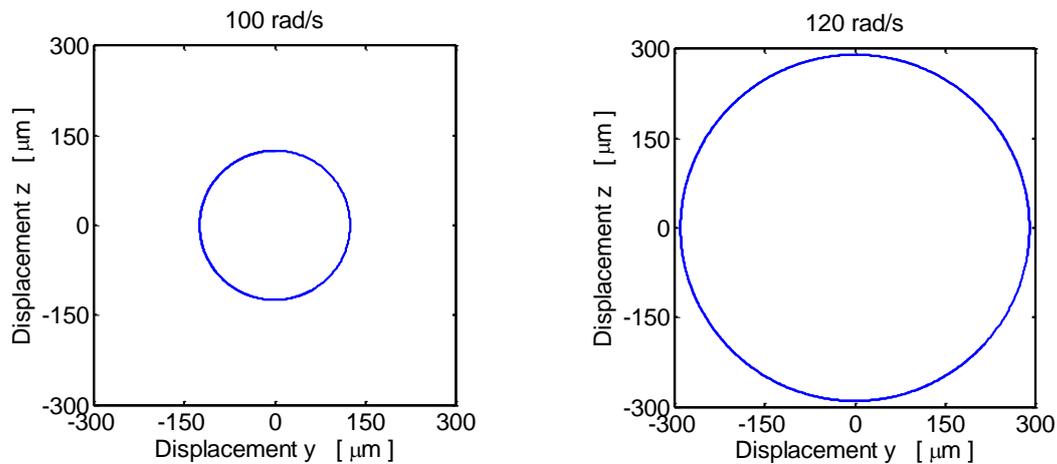


Fig. 4. The steady state orbits of the rotor centre for two running speeds (100, 120 rad/s) and no applied current.

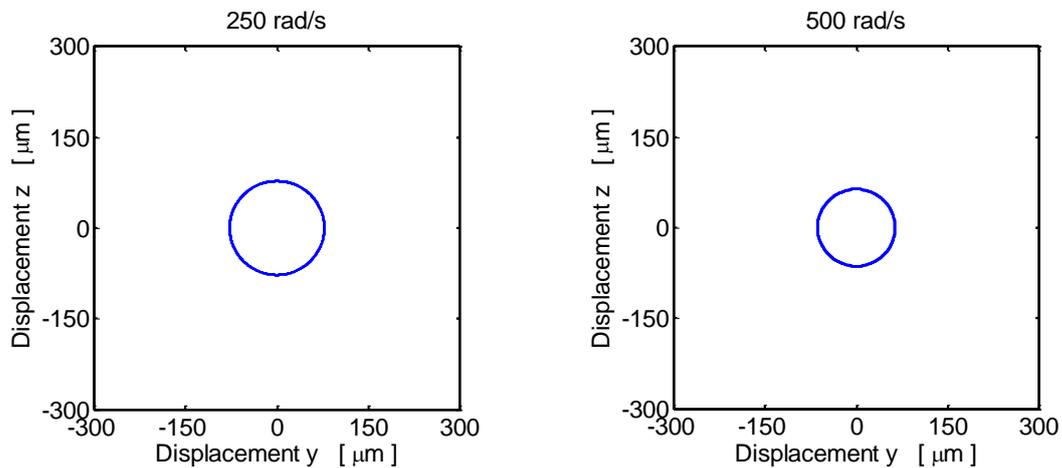


Fig. 5. The steady state orbits of the rotor centre for two running speeds (250, 500 rad/s) and no applied current.

The steady state orbits of the rotor centre for the case of zero applied current are drawn in Figs. 4 and 5. It is evident that the orbit reaches its maximum size for the speed of the rotor rotation close to the critical one and that the vibration amplitude of the rotor turning at speed

sufficiently higher than the critical one is close to the eccentricity of the rotor unbalance ($60 \mu\text{m}$).

The increase of the current feeding the coils of magnetorheological dampers for different speeds of the rotor rotation is drawn in Figs. 6 - 9. The results are related to the current (CC) and voltage (VC) control regimes. They show the time delay of the current history if the voltage control is applied.

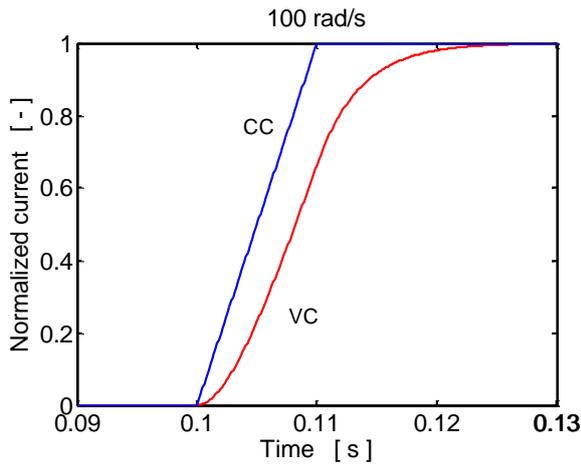


Fig. 6. Normalized current (100 rad/s).

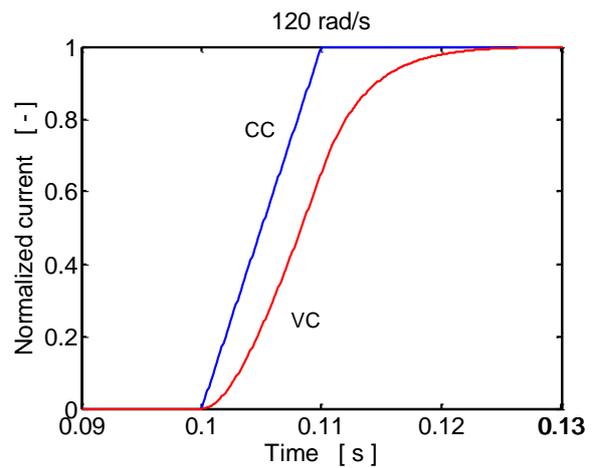


Fig. 7. Normalized current (120 rad/s).

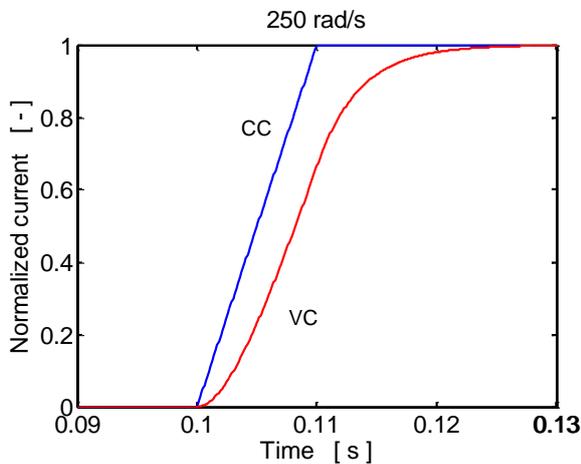


Fig. 8. Normalized current (250 rad/s).

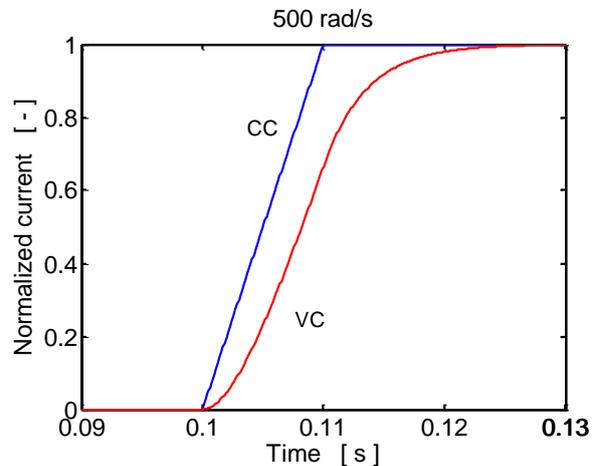


Fig. 9. Normalized current (500 rad/s).

Figs. 10 - 13 show the time history of the rotor centre eccentricity (the total rotor vibration amplitude) after increasing the damping effect in the rotor supports. The eccentricity goes down approximately in a monotonic way for the rotational speeds lower than the critical one while for higher angular speeds the time history of the eccentricity has an oscillatory

character. The delay of the rotor response is evident in all investigated cases if the damping is controlled by the change of voltage.

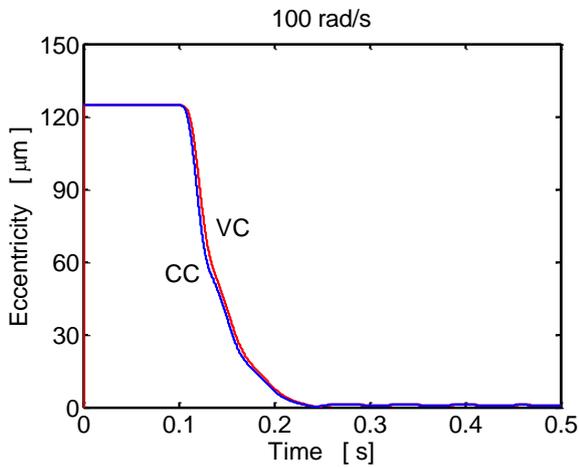


Fig. 10. The rotor centre eccentricity (100 rad/s).

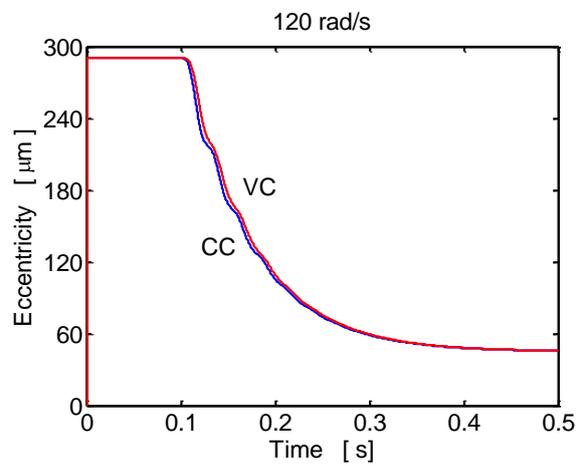


Fig. 11. The rotor centre eccentricity (120 rad/s).

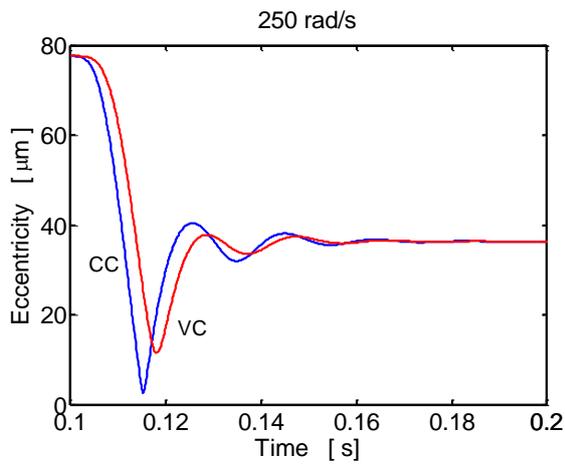


Fig. 12. The rotor centre eccentricity (250 rad/s).

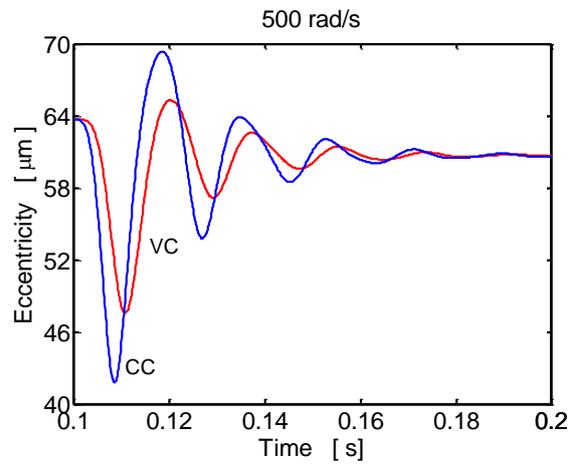


Fig. 13. The rotor centre eccentricity (500 rad/s).

The time histories of the normalized current (ratio of the instantaneous to desired current value) for the cases of the current and voltage control regimes and shorter time of rising the damping effect (1 ms) for two rotor rotational speeds are drawn in Figs. 14 and 15.

Figs. 16 - 17 show the corresponding rotor responses. The disturbance of the vibration (comparing with Figs. 12 and 13) is higher. The time delay of the rotor response if the damping effect is controlled by the voltage is evident. Maximum magnitude of the rotor centre eccentricity is higher if the current control strategy is used.

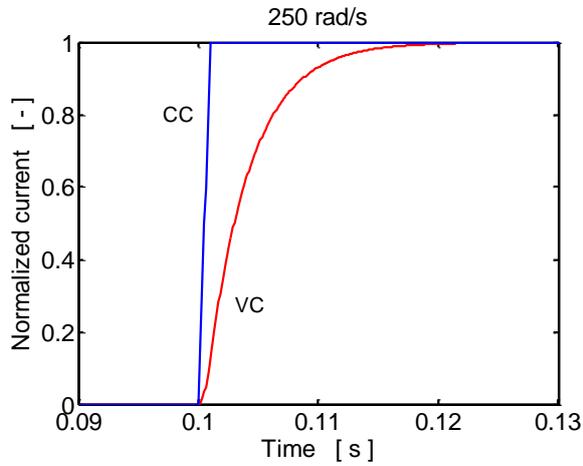


Fig. 14. Normalized current (250 rad/s, 1 ms action).

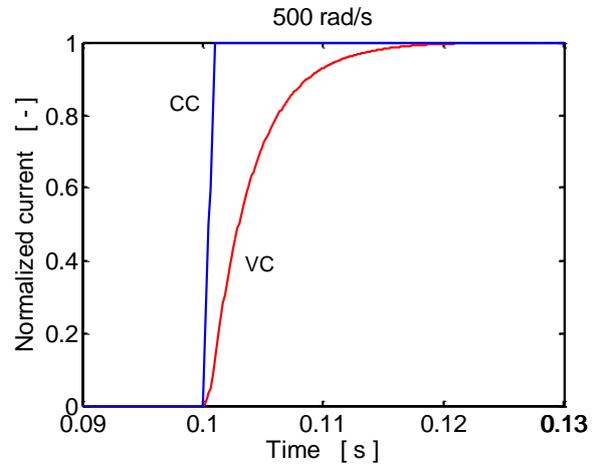


Fig. 15. Normalized current (500 rad/s, 1 ms action).

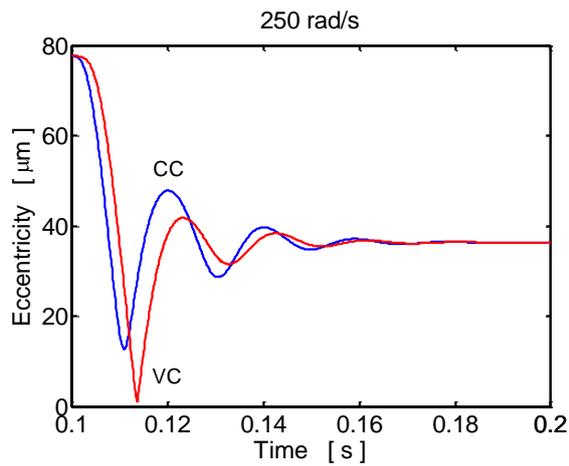


Fig. 16. The rotor eccentricity (250 rad/s, 1 ms action).

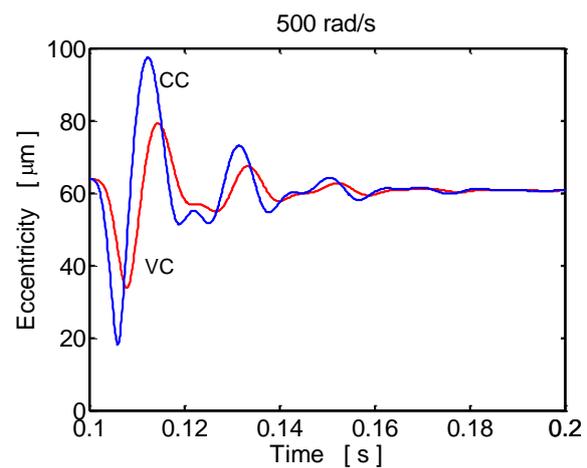


Fig. 17. The rotor eccentricity (500 rad/s, 1 ms action).

6 CONCLUSIONS

This paper presents an enhanced mathematical model of a short magnetorheological squeeze film damper and its utilization for comparing two strategies to control of the damping effect.

The new mathematical model is multiphysical. It takes into account the mutual interaction between the hydraulic forces, transient electromagnetic phenomena, and the mechanical vibration. Its development is based on assumptions of the classical theory of lubrication. The oil is represented by bilinear material. The pressure distribution in the full oil film in the damper gap is governed by the adapted Reynolds equation.

The damping force can be regulated either by means of the current or voltage control. The former controls the voltage with the aim to achieve the required time history of the current while the latter controls the voltage with the goal to achieve its required time course. It implies the voltage control strategy is technologically less complicated and thus more reliable than controlling the current. The efficiency of both strategies from the point of view of suppressing the rotor vibration was compared by means of computer simulations, during which the response of a rigid rotor excited by the unbalance was investigated. The results show that (i) the response of the rotor is faster if the current control is applied, if the voltage control is used, the response is delayed, (ii) in all investigated cases when the damping effect was controlled by the voltage the eccentricity of the rotor centre (the total amplitude of the rotor vibration) never exceeded the magnitude of the vibration when the current control was applied, and (iii) the disturbance of the vibration of the rotor running at angular velocity higher than the critical one was greater in the cases when the period of the manipulation action (the change of the voltage or current) was shorter and the disturbance did not depend on the damping control regime.

The development of the enhanced mathematical model of the magnetorheological squeeze film damper contributed to learning more on properties of magnetorheological damping devices and on their influence on vibration attenuation of rigid rotors.

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A Load Balance Strategy for Partitioned Multi-physics Applications

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ABSTRACT

One of the main challenges of multi-physics problems is the development of approaches and algorithms with the capability of solving efficiently large-scale problems on extreme scale architectures. An approach widely used to solve multi-physics applications is based on the partition of the computational domain into regions. Each of these partitions is governed by a particular physical field principle. In this approach, the solution of the whole domain can be reconstructed from each partition through an iterative coupling algorithm. The main drawback of this approach is related to the unbalance introduced when an inappropriate selection in the allocation of the available resources is done. The aim of this paper is to introduce and validate a load balance strategy for partitioned multi-physics applications which enables reaching an optimal parallel performance. As a result, it is possible to estimate the behaviour of the parallel performance metrics of any partitioned multi-physics application composed of two parallel partitions. Finally, the proposed strategy is applied to a conjugate heat transfer problem with up to 2048 CPU-cores where it is shown the validity of the approach.

Clever Mechanisms and Strategies Found in the Architecture of Some Naturally Occurring Materials

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ABSTRACT

There is a strong demand for new paradigms of design and development of advanced high-performance structural materials with high specific strength, stiffness and toughness for new technological needs. Yet, most engineering materials have an inverse relation between these desired properties. By natural selection, Nature has evolved efficient strategies to synthesize materials that often exhibit exceptional mechanical properties that significantly break the trade-offs often achieved by man-made materials. In fact, most biological composite materials achieve higher toughness without sacrificing stiffness and strength in comparison with typical engineering material. Interrogating how Nature employs these strategies and decoding the structure-function relationship of these materials is a challenging task that requires (i) knowledge about the actual loading and environmental conditions of the material in their natural habitat, (ii) a complete characterization of their constituents and hierarchical architecture through the use of modern tools such as in-situ electron microscopy, small-scale mechanical testing capabilities, and (iii) solving some interesting solid mechanics problems that involve analytical and numerical models, as well as additive manufacturing. This talk will be focused on the convergent evolution of impact resistant naturally occurring materials and how we can use computational tools and mechanics to evaluate some important hypotheses about the key morphological features of the microstructure and toughening mechanisms that are unique in these hierarchical materials.

SHAKING-TABLE TEST WITH HEAD-MOUNTED DISPLAY AND VIRTUAL REALITY TO QUANTIFY ANXIETY DURING STRONG MOTION

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Key words: Quantifying anxiety, Head mount display (HMD), Virtual reality (VR), Shaking table test, Questionnaire.

Abstract. In present-day Japan, not only structural reliability, but human safety and comfort during strong motion are important issues for structural engineering. Quantifying the level of anxiety that occurs during strong motion is valuable for clarifying the structural performance needed for human comfort and will facilitate the communication between structural designers and clients about risk. In this study, a shaking-table test for humans who are wearing a head-mounted display (HMD) was performed to quantify the levels of anxiety during strong motion. To determine the influence of falling furniture during strong motion, a scenario consisting of a living room with several pieces of furniture was also simulated using virtual reality (VR). The vibration period, speed, and shape of the input motion were varied for each VR-based situation. The results of the test show that a longer shaking period produced lower levels of anxiety. View direction, which changed the direction in which the television and bookshelf fell relative to the participant, was observed to affect levels of anxiety, but these results are limited. The results of this study will further advance our understanding about how vibration in a building affects the anxiety of its occupants during earthquake events.

1. INTRODUCTION

In present-day Japan, not only structural reliability, but human safety and comfort during strong motion are important issues for structural engineering. When earthquakes occur, evaluating the ability to evacuate according to factors such as human psychology and falling furniture is very important for ensuring indoor safety. In past studies that looked at the injuries that occurred during a magnitude 7 earthquake, the proportion of injuries due to falling furniture was higher than those caused by the collapse of the building [^{1,2}]. Moreover, human behavior is related to the movement of furniture in such situations [³]. Therefore, quantifying anxiety during strong motion is valuable for clarifying the structural performance needed for human comfort and facilitates the communication between structural designers and clients about risk. In this study, a shaking-table test for humans using a head-mounted display (HMD) was performed to quantify anxiety during strong motion. To evaluate the influence of falling furniture during strong motion, virtual reality (VR) was used to simulate a living room with a table, sofa, chairs, television, bookshelf, and sideboard during strong motion. The aim

was to assess the difference in the level of anxiety experienced by subjects using a shaking table and an HMD that displayed two different views of a virtual scene in which the furniture either fell to the side or forward with respect to the observer under the same vibration [4,5,6].

2. SHAKING-TABLE TEST

The shaking-table tests were performed from Nov 8th to Dec 15th, 2017. We conducted experiments on 15 subjects (all males), using a simple vibration table installed in the Building Engineering Laboratory at Chiba University, Japan. We asked subjects to answer a questionnaire after experiencing multiple excitations that were presented with two different views of a virtual scene of falling furniture, displayed under the same vibration conditions. In each experiment, the subject's bioinformatics were measured and the acceleration was measured by accelerometers attached to the shaking table and one subject's head.

2.1 HMD

While they experienced the vibration of the shaking table, the subjects wore an HMD (Fig. 1) that displayed a virtual scene synchronized with the vibration to simulate an actual earthquake situation. Each virtual scene shows the two directions in which furniture tends to fall: along the x-direction, i.e., side to side (room x; Fig. 2) and along the y-direction, i.e., forwards and backwards (room y; Fig. 3).



Fig. 1 HMD and experimental setup



Fig. 2 Virtual scene in which furniture collapses in the x direction (room x): (left) before and (right) after vibration.



Fig. 3 Virtual scene in which furniture collapses in the y direction (room y): (left) before and (right) after vibration.

2.2 Vibration Waves and Inputs

In the tests, six vibration periods (0.4, 0.6, 1.0, 2.0, 3.0, and 4.0 s), four levels of input motion (0.1, 0.15, 0.3, and 0.6 m/s), and five input directions (x-direction, y-direction, O-shape, 8-shape, and ∞ -shape) were performed for each viewpoint of the virtual scene. However, some of these inputs were abandoned because of the limitations of the stroke and maximum acceleration of the vibration table. Therefore, each participant was subjected to a total of 142 inputs in this experiment. Vibration was continued for a duration of 12 to 32 s, and the excitation sequence was random to take into account the psychological impact on the subject. The magnitude of the internal change has a significant impact on three indoor conditions: whether the bookshelf falls, the television falls, or the table falls.

2.3 Questionnaire

The subjects were asked to answer a questionnaire after each shaking-table vibration was completed. The questionnaire evaluated three main aspects: the degree of anxiety (on a scale from 0 to 4), ability to take action (on a scale from 0 to 2), and sense of shaking (“forward and backward,” “side to side,” or “not sure”). The questions are shown in Table 1.

Table 1. Questionnaire

(A) How did you feel in the shaking table experiments? (Degree of anxiety)	
0. I had no anxiety.	1. I felt a little anxiety.
2. I felt anxiety.	3. I felt some anxiety.
4. I felt a lot of anxiety.	
(B) Do you think you could take action if it were the real earthquake? (Ability to take action)	
0. I can take action.	1. I am not sure whether I can take action or not.
2. I do not think I can take action.	
(C) Which shaky feeling is stronger, when the furniture falls side to side or forward and backward under the same vibration?	
0. I felt more strongly forward and backward.	1. I am not sure.
2. I felt more strongly side to side.	

3. TEST RESULTS

3.1 Questionnaire analysis method

The results of the questionnaire after each input motion are presented in this paper. In the bubble charts in Fig. 4, the horizontal axis is the maximum input speed of and the vertical axis indicates the score of the questionnaire item. The size of the bubble is related to the number of subjects who gave that answer. Finally, a straight line was fitted to the data using the weighted least squares method. In this study, we focus on the degree of anxiety in the questionnaire results.

3.2 Comparison of Room x and y

In general, the results for the four periods (0.4, 0.6, 1.0, and 2.0 s), fluctuate substantially, while the effects of environmental changes are small and the virtual scene is not much different at 3.0 s and 4.0 s (Fig. 4).

First, we compare the x-direction with the 8-shaped vibration patterns in room x, which creates large changes in the room. At 15 cm/s speed, which has no effect on the indoor environment, more people in room x have a high degree of anxiety during short-period vibrations and more participants have a high level of anxiety in room y during long-period vibrations, depending on the video. It is hard to determine how anxiety is influenced by the video. However, in the case of large indoor changes at 60 cm/s, there are many participants with a high level of anxiety in all rooms except during the x-direction vibration with a period of 0.4 s. In particular, there is an especially big difference between the 1.0 and 2.0 s of the 8-shaped vibration cycle. All other results differ by about one or two people.

Next, we compared the effects of y-direction and vibration patterns in room y with large variations. At the 15 cm/s rate, there was no effect on the indoor environment for the y-direction periods of 0.4, 0.6, 1.0, and 2.0 s and the ∞ -shape periods of 0.4 and 1.0 s. Room x generated a high degree of anxiety for ∞ -shape motion with a period of 2.0 s. The number of people with high anxiety in room y was high, and this number did not change according to the

video. It is also difficult to determine the influence on these results. However, when indoor changes are affected by speeds as high as 60 cm/s, except for the ∞ -shape period of 0.6 and 2.0 s, all other conditions in room y lead to high levels of anxiety. Here, there is also a difference in answers of about 1 or 2 people.

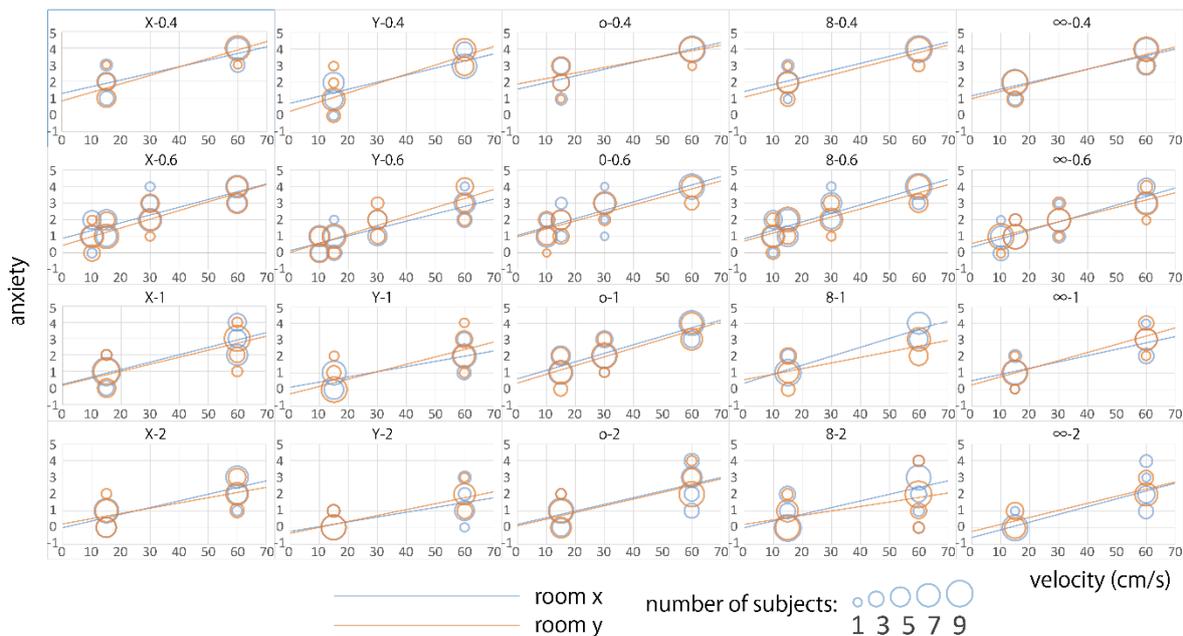


Fig. 4 Degree of anxiety for each virtual scene

Finally, for the o-shaped vibration pattern of the same degree in rooms x and y, the number of participants with high anxiety in room x are high at 0.4 s and 15 cm/s. Moreover, many participants had high anxiety in room x.

To summarize these results, it is very difficult to determine the change in discomfort based on a comparison of the virtual scene only because of the small number of test subjects. However, an individual's anxiety level has a large impact on the changes in the chart. Regardless, there are some effects at a speed of about 60 cm/s or more; the results show that there is some influence on the degree of anxiety.

3.3 Performance evaluation curve

From the questionnaire results, we determined an approximate curve corresponding to the anxiety evaluation values and speeds depending on the different types of vibrations and periods. Considering the full cycle, we plotted the period using the horizontal and vertical axes for each evaluation. By performing this operation for each vibration shape, a performance evaluation curve is obtained (Fig. 5).

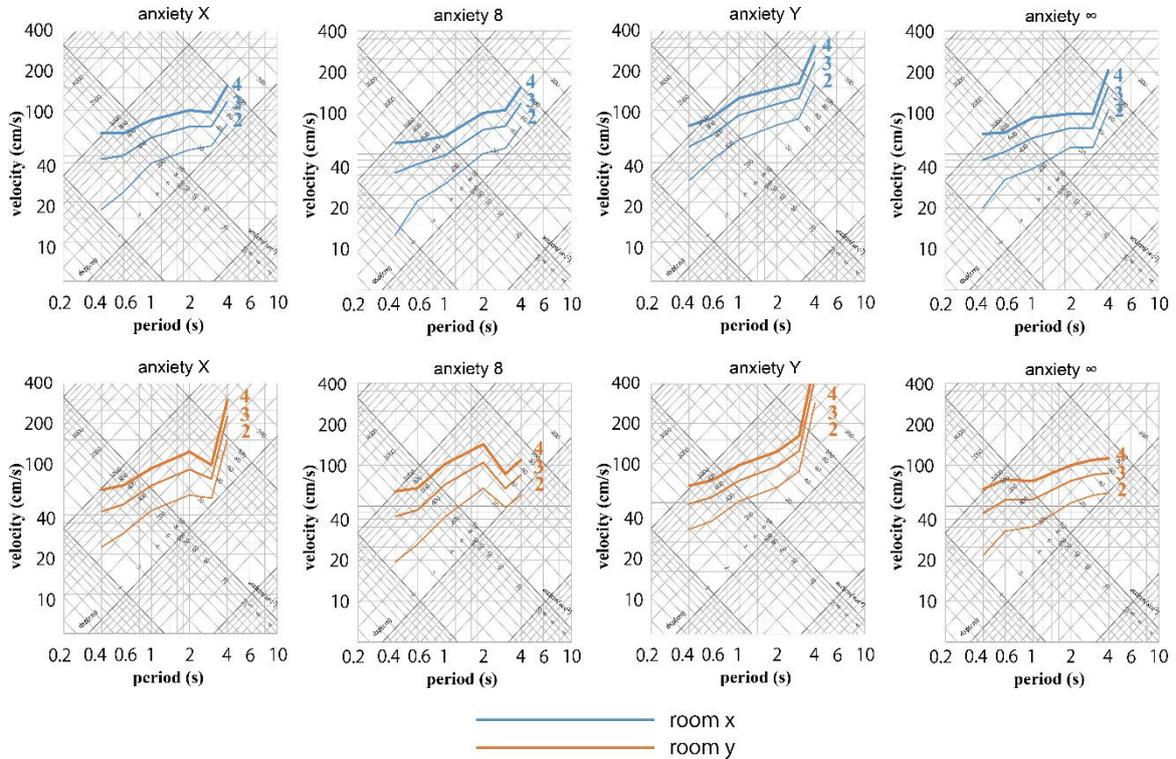


Fig. 5 Comparison of performance evaluation curves

First, room x has a lower curve than room y when comparing the x-direction and 8-shape graphs. In other words, room x is more likely to make people feel anxious. Second, comparing the y-direction with ∞-shape graphs, the room y has a lower curve than room x. In other words, room y is more likely to make people feel uneasy.

Thus, based on a comparison of the performance evaluation curves, we believe that the virtual scenes have an effect on the degree of anxiety. However, compared with the results in Fig. 4, because the influence of each anxiety level is large and the difference in the performance evaluation curve is small, it is difficult to precisely describe the effect of the virtual scene.

3.4 Comparison of the conclusions of the previous result

Using fitted lines, we compare the results for room x and y in 2017 with the results obtained in Oct 13th to Nov 15th, 2015 and Feb 15th to Mar 14th, 2017 [7]. We used the same oscillation conditions, vibrations at speeds of 10, 15, 30 and 60 cm/s, and 0.6 s (Fig. 6).

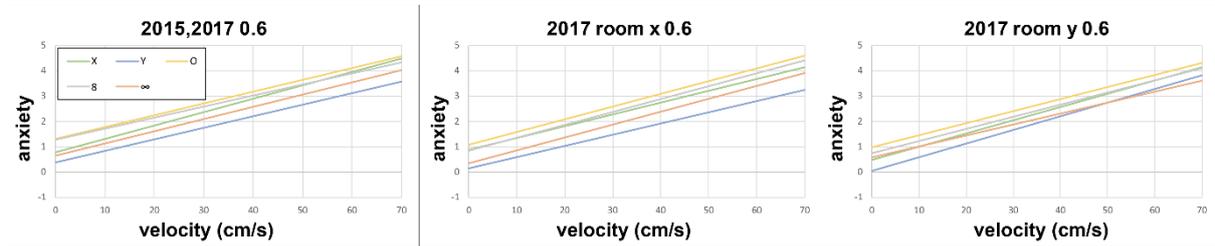


Fig. 6 Comparison of the results from 2015 to 2017.

In all charts, the O-shape vibration generates the highest degree of anxiety. This is thought to be due to the centrifugal sensation that the O-shape vibration produces, which is like a smooth circle. The O-shape vibration does not create a very different variation in the condition of each virtual scene, and the virtual scene appears to have no special influence on the results. Therefore, regardless of which room is used in 2017, any virtual scene will cause participants to feel very uncomfortable. Moreover, the x-direction vibration excitation generates a greater degree of anxiety than the y-direction vibration excitation. This is because the experiment is performed on a chair with a leg structure that can alleviate the impact of the subject's shaking. In contrast, there is no support in the left and right directions. Alternatively, it may be that when people first sit in a chair and receive vibrations, the side-to-side shakes are more likely to cause anxiety than forward-and-backward shaking. In room y, the x-direction vibration with less indoor variation generates more anxiety than the y-direction vibration with greater indoor environment variation and is not affected by the virtual scene. Alternatively, it could be that despite the influence of the virtual scene, the influence of the direction of vibration is greater.

4. CONCLUSIONS

The results of this experiment show that indoor changes may have an impact on people's anxiety. In addition, it is necessary to note the difference in the degree of anxiety between the x-direction vibration and the y-direction vibration. However, because the total number of experimental data is still very small, these results may not be very accurate. In future, the number of experiments and the total number of data should be increased.

In addition, it is necessary to verify the reliability of this conclusion from various viewpoints of these data, such as the ability to take action, the strong sense of shaking direction, biological information, and acceleration.

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Analysis of Nonequilibrium Scale Effects in the Shock Wave-Boundary Layer Interactions

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ABSTRACT

Abstract? Reduced scale models are generally used in the laboratory simulation of flow with shock wave-boundary layer interactions. If chemical reactions take place in the flow, it is important to take into account of the nonequilibrium scale effects which result from the finite rate of the chemical kinetics. The simulated parameter of scale effects is the product of free stream density ρ_0 and the characteristic length L ($\rho_0 L$, binary scaling parameter) for dissociation nonequilibrium flow and $\rho_0^* \rho_0^* L$ for recombination nonequilibrium flow, while for equilibrium or frozen flow, there are not scale effects except for those result from viscosity. For hypersonic flow over blunt body where the binary dissociations are dominant behind the detached bow shock, the binary scaling parameter $\rho_0 L$ can simulate the nonequilibrium scale effects, and at the same time the Reynolds number which embodies the viscous effects can also be sufficed. However, for the flow with shock wave-boundary layer interactions, the three-body recombination reactions can not be neglected in the boundary layer near the cold wall. Moreover, if the flow separation occurs, the recombination reactions may be comparable with dissociation reactions in the separation zone. Therefore, the nonequilibrium scale effects are somewhat complex for the shock wave-boundary layer interaction flow, and the simulation parameter for nonequilibrium scale effects for the flow should be investigated further. Taking the shock tunnel test model, a two dimensional compression corner (with total length of 0.6096m and the front plate length of 0.3048m) as the base one, the flow over models with 2 and 5 times scales are all simulated numerically for the analysis of the nonequilibrium scale effects. Twelve free stream conditions are selected with speed range from 3000 to 6000m/s and the values of $\rho_0 L$ range from 0.003 to 0.03 kg/m². The hypersonic nonequilibrium compression corner flow for three corner angles (15, 18 and 24 degrees) and three different model scales are numerically simulated. The behaviour of nonequilibrium scale effects on the flow structure and separation properties are analyzed for the various free stream conditions which corresponding to various flow thermochemical states. Through combining the numerical analysis and Triple Deck theory in the analytical treatment of shock wave boundary layer interactions, the similarity law for nonequilibrium flow is studied, the determination of nonequilibrium scale effects simulation parameter as well as its validity range is investigated.

key words? nonequilibrium flow, nonequilibrium scale effects, compression corner flow, flow separation, numerical simulation

The Evaluation of Reverse Shoulder Lateralization on Scapular Fracture Risk: a Computational Study based on Different Failure Criteria

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ABSTRACT

As an effective solution for patients with glenohumeral joint disease, reverse shoulder arthroplasty (RSA) can treat severe rotator cuff deficiency, but its medialization design of the shoulder's center of rotation (CoR) has been associated with scapular notching caused by impingement. Recent studies have shown that lateralization has beneficial effects on decreasing of notching and improving rotational capability in RSA. However, few studies have quantified the relationship between fracture failure risk of scapular and the specific design variations, especially lateralization. In this work, we estimated the impact of glenosphere lateralization to scapular strain/stress state by computational modeling, which can identify potential risk of scapular fracture. The comparison study showed larger lateralization produced higher strain/stress concentrations in scapular spine (Levy Region Type II), with approximately 10% increase for 12 mm lateralized loading scenario. The FE results were analyzed using three most representative failure measures. The occurrence of fracture risk predicted by maximum principal strain behaved similarly as the maximum principal stress measure since the bone was assumed to be isotropic. However, the largest area of high fracture risk predicted using von Mises stress measure identified a different risk pattern. Studying the effects of RSA lateralization on scapular fracture risk can help guide continued optimization of RSA performance and surgical techniques. The findings on the connections between loading style and bone failure measures can provide valuable insight into future research on the assessment and improvement of the generality of bone failure criteria.

Embedded Boundaries in ALE Flow Computations for Shock Hydrodynamics and Multi-Fluid Simulations

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ABSTRACT

We present a computational framework that combines an embedded boundary method and an arbitrary Lagrangian-Eulerian (ALE) method for multiphase flow computations of compressible fluids. This methodology is capable of handling geometrically complex material interfaces on moving grids and is suitable for multi-material flow computations in the context of ALE shock hydrodynamics. Specifically, we use a variational multiscale stabilized finite element method to update the fluid state of each material, and define ghost values to enforce the transmission condition at the embedded material interface, which is captured using a level-set approach. Two different strategies to populate ghost values are considered and compared, namely the constant extrapolation and a multi-material Riemann solver. The accuracy and conservation properties of both ghost value population strategies are assessed using benchmark shock tube problems and blast/bubble interaction problems. The method is then extended to solve multi-fluid problems with more than two fluids such as the triple-point problem, where multiple material interfaces are captured by the projected level set method; and it is also extended for numerical simulation of a liquid-gas-solid interaction problem, where body-fitted grids are used to track the multi-fluid/solid interface and an embedded boundary separates the liquid from the gas.

Numerical Investigation of the Role of Cell-Cell Interactions on Cell Locomotion in a Tightly Packed Epithelial Monolayer Sheet

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ABSTRACT

In epithelium, cells are tightly anchored and attached to each other through cell-cell adhesions. Forces exerted between cells determine tissue homeostasis as well as reorganization during embryonic development, wound healing and disease development. To understand how cell-cell interaction forces will influence the tissue state, we develop a novel vertex based simulation model for adhesive cell clusters and monolayers. In this presentation, we shall present our latest results on cell locomotion in a tightly packed epithelial monolayer sheet based on cell growth, division, remodeling and migration. In the simulation, a 2D epithelial monolayer sheet was generated. The macroscale cell is modeled as soft materials, and cell-cell/substrate interactions are governed by a recently developed interfacial zone model. The polygonal shape of epithelial cells is generated using Voronoi tessellation techniques. We have developed and implemented the related computational algorithms into simulation code for the described cell growth, division, remodeling and migration model. The simulation shows that the cell locomotion depends on cell-cell interaction, and the stronger cell-cell adhesion may play a role on "jammed" state in an epithelial cell cluster.

Derivation of Conical Indentation Model for Hyperelastic Materials Assisted by Dimensional Analysis and Finite Element Analysis

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ABSTRACT

Classical conical indentation model, which is based on linear elastic assumption, is not suitable to extract mechanical parameters of hyperelastic materials for the following two reasons. Firstly, the parameter obtained from classical model is not accurate when dealing with single-parameter hyperelastic materials, because hyperelasticity is not considered in the model. The error will be larger if the half angle of the conical indenter is small, because hyperelasticity will significantly violate the linear elastic assumption under sharp indenters. Secondly, because classical model can provide only one material parameter, it's not capable to deal with double-parameter hyperelastic materials. Moreover, it is mathematically impossible to extract the parameters of double-parameter hyperelastic materials through single indentation experiment, no matter what model is used, because the uniqueness of the parameters can't be guaranteed. To solve the above two problems, dimensional analysis and finite element analysis are applied in this work. Dimensional analysis is to construct the mathematical form of conical indentation model. To solve the non-unique problem, dual-indenter method is adopted and the mathematical form of the corresponding indentation model is also constructed by dimensional analysis. Finite element analysis is to determine the model parameters in the constructed models. Because severe element distortion will be induced by conical indenter during finite element analysis, re-meshing processes are inserted in simulation to obtain accurate results. After constructing the indentation models, the stability of the models are analyzed. Conical indentation models for single- and double-parameter hyperelastic materials were constructed in this work. By adopting the models, conical indentation experiment, which is simple to conduct and can obtain local property of material, can be applied to capture mechanical properties of hyperelastic materials.

Numerical Simulation of Underwater Contact Explosion Based on the Coupled SPH-FEM Method

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ABSTRACT

It often brings deadly threat to the warship subjected to underwater contact explosion. Therefore, studies on the load characteristics and damage mechanism are of great significant. The loads of contact explosion consist of shock waves, high-velocity fragments, water-gas jet induced by detonation, bubble jet, etc., which are characterized by high temperature, high pressure and high speed shocks, and accompanied by large deformation, tearing, attacking, and splashing and so on, which makes it hard to solve with traditional mesh-based method. As a meshless particle method, the smooth particle hydrodynamics (SPH) can easily track the moving interface and well deal with the large deformation problems. Thus, the coupled SPH-FEM method is employed to simulate this phenomenon in this paper. In the present work, a novel nonreflecting boundary condition is proposed to economize calculating time, and the Riemann-solver is adopted to reduce the pressure oscillation at the interface of water and detonation products. The numerical results are compared with experimental or theoretical results to validate the applicability of the current procedure. Furthermore, the load characteristics of contact underwater explosion and the damage mechanism of the nearby ship structures are studied, which provides some references for the structural design of naval architecture of underwater explosion. Key words: SPH-FEM; Underwater contact explosion; Nonreflecting boundary; Riemann-solver Reference: Zhang A, Wen-shan Y, Xiong-liang Y. Numerical simulation of underwater contact explosion[J]. Applied Ocean Research, 2012, 34: 10-20. Liu M B, Liu G R, Lam K Y, et al. Smoothed particle hydrodynamics for numerical simulation of underwater explosion[J]. Computational Mechanics, 2003, 30(2): 106-118.

Numerical Simulation of Mechanical-electrical-thermal Failure for Lithium-ion Batteries under Impact Loads

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ABSTRACT

Crashworthiness and mechanical crash induced internal short circuit are critical concerns for the deployment of lithium-ion batteries on electrical-driven vehicles. In this work, we intend to investigate mechanical failure, the initiation of short circuit and the propagation of thermal events for lithium-ion battery cells under impact loads. The lithium-ion cell can be considered as a multi-layer stacked structure made of anodes, cathodes and separators. To model it, we introduce a multi-scale approach to solve the stress status of each component while treating each battery cell as a homogenized layer in macro scale. Extensive tensile and compressive tests are conducted to characterize the basic mechanical properties of each cell component, which are implemented into the multi-scale model through a user-defined material model. Also, experimental results of single battery cell are used to validate the material model. We build the model using the mechanical solver and Multiphysics solver of finite element software LS_DYNA. The stress history is utilized to predict the mechanical failure for each representative element of the battery cell and to calculate electrical contact resistance based on the failure status of cell components. The coupled mechanical-electrical-thermal failure (including force response, voltage response and temperature history profiles) of a pouch lithium-ion battery cell under impact is then studied numerically and compared with experimental results. Through numerical parameter study, we elaborate the effect of impact conditions on the consequential failure behavior of battery cells, and highlight important physical properties that impacts the coupled responses. The results and modeling approach presented in this study form the basis for safety studies of lithium-ion batteries, and are especially useful for the design and optimization of battery structures for electrical-driven vehicle applications.

Bi-directional Coupling between a PDE-domain and an Adjacent Data-domain Equipped with Multi-fidelity Sensors

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ABSTRACT

We consider a new prototype problem in domain decomposition with the solution in one domain governed by a known partial differential equation (PDE) whereas in an adjacent domain the solution is reconstructed by information gathered via distributed sensors (data) of variable fidelity. The PDE-domain and the Data-domain are tightly coupled, as the PDE solution is driven by the collected data, while the information gathered from its associated network sensors is influenced by the PDE solution. Our overall methodology is based on the Schwarz alternating method and on recent advances in Gaussian process regression (GPR) using multi-fidelity data. The effectiveness of the proposed domain decomposition algorithm is demonstrated using examples of Helmholtz equations in both 1D and 2D domains.

Multifield Formulation for Fluid-structure Interactions

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ABSTRACT

Interface tracking and reconstruction methods are used often for fluid-structure interaction problems. Most of these methods start with some initial interfaces. However, there are cases where material interfaces are not known a priori. The examples range from crack or spall surface formation under impact loading to flaking of mud in a slowly drying puddle. This presentation introduces a fully coupled numerical scheme for material interactions, in which the material locations and the interfaces are described by the volume fraction fields of the materials. The numerical scheme is based on the ensemble phase averaging method. Interactions among the materials are considered through the closure relations of the averaged equations. This treatment of the material interactions has an additional advantage that the equations are applicable to material interactions occurring inside body of the materials, such as fluid-solid interactions in a porous material. Interactions on the material interfaces are treated in the same manner as the body interactions. No special treatment for interfaces is necessary. Numerically, the equations for the solid material are solved using the dual domain material point method, which uses Lagrangian points to track history dependent state variables, such as damage, failure, and plastic strain of the solid. The distribution of the material points provides natural description of the material locations and interfaces. The material point method also uses Eulerian description for the material. In the numerical scheme described here, the Eulerian description is used to couple with the calculation of fluids. To ensure consistence of the Lagrangian and Eulerian descriptions, a weak solution method is introduced to enforce the continuity condition. The numerical method is shown to be quite versatile. Many advanced material models can be implemented to study complex fluid-structure problems with large deformations of the solids. After reviewing basic concepts of the material point method and its recent advances, I will present examples of crack formation in a ductile material subjected to blast loading using a rate-dependent tensile plasticity model [1,2]. This work was performed under the auspices of the United States Department of Energy. [1] J. Johnson, F. Addessio, Tensile plasticity and ductile fracture, *J. Appl. Phys.* 64 (12) (1988) 6699–6712. [2]. F. L. Addessio, J. N. Johnson, Rate-dependent ductile failure model, *Journal of Applied Physics* 74 (1993) 1640–1648.

3D Tensor Field Design

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ABSTRACT

Hexahedral mesh generation is a delicate process. Recent advances in the area make use of a 3D frame field to guide the orientation of the mesh elements. In this talk, we will explore the design of 3D tensor fields, which can be used as a frame field. We will discuss how to control the smoothness of the tensor field as well as its topological structures, which have implications in controlling the irregular vertices in the resulting mesh.

A Multi-material Topology Optimization Method for Energy Absorbing Designs with Viscoelastic and Hyperelastic Materials

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ABSTRACT

Energy absorbing designs are of great importance in many engineering applications. Traditional experimental/experience based design methods for such applications are time consuming, however. As an alternative, topology optimization (TO) can be used as a conceptual design method. As desired in practical applications, energy absorbing designs should have optimal energy absorbing capacity together with necessary stiffness. To achieve this objective, a multi-material TO considering finite deformation is presented in which a viscoelastic material – that provides dissipation – is combined with a hyperelastic material – that provides stiffness. Several issues pertaining to the multi-material design framework are discussed and addressed. In particular, for the developed multi-material density-based TO, a material interpolation scheme is proposed for mixing viscoelastic and hyperelastic phases. Besides, due to the use of incompressible viscoelastic material, F-bar formulation is adopted to handle the volumetric locking. Moreover, a constitutive model interpolation approach is proposed to address the mesh distortion issue induced by the use of fictitious domain in TO. Finally, an analytic path-dependent adjoint sensitivity analysis is given that is necessary for gradient-based optimizers. The proposed framework is demonstrated to be effective through several numerical examples.

Uncertainty Quantification and Propagation of Imprecise Probabilities with Copula Dependence Modeling for Composite Material Properties

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ABSTRACT

Abstract Imprecise probability, as a generalized probability theory, allows for partial probability specifications and is applicable when data is so scarce that a unique probability distribution cannot be identified. The primary research challenges in imprecise probabilities relate to quantification of epistemic uncertainty and improving the efficiency of uncertainty propagation with imprecise probabilities – particularly for complex systems in high dimensions, at the same time considering dependence among random variables. The conventional method to address variable dependence from limited information is to assume that the random variables are coupled by a Gaussian dependence structure and rely on a transformation into independent variables. This assumption is often inaccurate, subjective, and not justified by the data. A novel UQ methodology has been recently developed by the authors [1, 2] for quantifying and efficiently propagating imprecise probabilities with independent uncertainties created by the scarcity of data. In this study, we generalize this novel UQ methodology to overcome the limitations of the independence assumption by modeling the dependence structure using imprecise vine copulas theory [3]. A data-driven Bayesian approach is investigated to quantify the uncertainties of copula dependence modeling for two composite material models with different dependent structures, including E-Glass fiber/LY556 Polyester Resin model and AS4 Carbon fiber/3501-6 Epoxy Resin model. The generalized approach achieves particularly precise estimates for uncertainty quantification and efficient uncertainty propagation of imprecise probabilities in copula dependence modeling for composite material properties. References [1] Jiixin Zhang and Michael D. Shields. On the quantification and efficient propagation of imprecise probabilities resulting from small datasets. *Mechanical Systems and Signal Processing* 98 (2018): 465-483. [2] Jiixin Zhang and Michael D. Shields. The effect of prior probabilities on quantification and propagation of imprecise probabilities resulting from small datasets. *Computer Methods in Applied Mechanics and Engineering*, 2017. (In Review) [3] Harry Joe. *Dependence modeling with copulas*. CRC Press, 2014.

3D Microstructure-based Finite Element Modeling of Deformation and Fracture of SiCp/Al Composites

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ABSTRACT

The mechanical behavior, with particular emphasis on the damage mechanisms, of SiCp/Al composites was studied by both experiments and finite element analysis in this paper. A 3D microstructure-based finite element model was developed to predict the elasto-plastic response and fracture behavior of a 7vol.% SiCp/Al composite. The 3D microstructure of SiCp/Al composite was reconstructed by implementing a Camisizer XT particle size analysis device and a random sequential adsorption algorithm. The constitutive behavior of the elastoplastic-damage in the metal matrix, the elastic-brittle failure for the particle reinforcement, and the traction-separation for interfaces, were independently simulated in this model. The validity of the modeling results were validated by the agreement of the experimental stress-strain curve and the morphology of fracture section with those predicted by the simulation. The visual elasto-plastic deformation process, along with crack generation and propagation was well simulated in this model. The numerical results were used to provide insight into the damage mechanisms of SiCp/Al composites, and the effects of interfacial strength and particle strength on material properties were also discussed in detail.

Accuracy Analysis of a Composite Implicit Time Integration Scheme and Application to Linear and Nonlinear Structural Dynamics

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ABSTRACT

The concept of two sub-steps composite implicit time integration scheme is extended in a generalized manner. A rigorous accuracy analysis in acceleration, velocity and displacement is performed, and the presented and proved accuracy condition enables the displacement, velocity, and acceleration achieving second-order accuracy simultaneously. The numerical dissipation and dispersion and the initial magnitude errors from the algorithmic amplification matrix's eigenvalues and eigenvectors are investigated physically. An optimal algorithm-Bathe composite method is revealed with unconditional stability, no overshooting in displacement, velocity, and acceleration and excellent performance compared with many other algorithms. The composite time integration scheme applying to linear and nonlinear structural dynamics cases is also performed, especially to solving the nonlinear dynamics problem of shell structures by combining the degenerated shell finite element method. References [1] Jie Zhang, Yinghua Liu, Donghuan Liu. Accuracy of a composite implicit time integration scheme for structural dynamics. *International Journal for Numerical Methods in Engineering*, 109(3): 368-406, 2017. [2] Jie Zhang, Donghuan Liu, Yinghua Liu. Degenerated shell element with composite implicit time integration scheme for geometric nonlinear analysis. *International Journal for Numerical Methods in Engineering*, 105(7): 483-513, 2016. [3] Klaus-Jürgen Bathe, Mirza M. Irfan Baig. On a composite implicit time integration procedure for nonlinear dynamics. *Computers & Structures*, 83(31-32): 2513-2524, 2005.

Automatic Polyhedral Mesh Generation for Scaled Boundary Finite Element Analysis

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ABSTRACT

Mesh generation of geometric models is an imperative task in the finite element analysis. Presently, the mesh generation process requires frequent human interventions, which are time consuming and error prone. Possible flaws and defects in the geometric models further increase the difficulty in mesh generation. It is recently shown that the polyhedral element formulated in the scaled boundary finite element method provides a higher degree of flexibility in mesh generation than standard finite elements [1]. This type of polyhedral elements may have arbitrary number of nodes, edges and faces. Only boundary discretization is required. What's more, a polyhedron doesn't need to be closed, leading to a convenient and accurate way to model concave shapes. In this paper, an automatic polyhedral mesh generation method is developed based on a modified octree scheme and Laplacian smoothing. A special technique is proposed to handle concave corners in the model. The steps of the proposed method are illustrated as follows. A uniform background grid is generated to cover the 3D model. The grid is refined on the surface of the model until a specified resolution is reached. The octree grid is trimmed by the surface so that a conforming mesh of arbitrary polyhedral elements can be generated. The mesh near the surface is optimized using Laplacian smoothing. The nodes on corners of the geometric model will not be moved during smoothing while the nodes on edges can be moved on the same edges only. The mesh quality can be significantly improved and sharp features are preserved. When a polyhedron containing concave corner is detected, a so-called scaling center is defined at the concave corner. This type of concave polyhedral elements can be analyzed directly by the scaled boundary finite element method. It improves the stability in mesh generation as well as the accuracy in stress analysis. Volume discretization is not required in the scaled boundary finite element method. Several numerical results are presented to verify the proposed method. [1] Liu, Y., Saputra, A. A., Wang, J., Tin-Loi, F., & Song, C. (2017). Automatic polyhedral mesh generation and scaled boundary finite element analysis of STL models. *Computer Methods in Applied Mechanics and Engineering*, 313, 106-132.

Reconstruction of Microstructure and Mechanical Properties of Short Fiber-reinforced Thermoplastic Considering Fiber Orientation and Length Distribution

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ABSTRACT

Accurate predictions of mechanical properties are of primary importance for the application of short fiber reinforced thermoplastic composites. Microstructure features are neglected for traditional methods when calculating effective elastic properties. In this study, we employed a random sequential adsorption algorithm to generate a representative volume element (RVE) based on fiber orientation distribution function (ODF) reconstructed by second-order fiber orientation tensor, which simulated the material microstructure of short fiber reinforced thermoplastic composites. Meanwhile, we performed finite element analysis on RVE samples with a homogenization procedure in parallel to evaluate the effective elastic properties of the whole composite. The illustrative example demonstrated that reconstructing ODF can predict precisely elastic properties compared to traditional methods. Furthermore, a modified random sequential adsorption algorithm was proposed to generate a RVE based on ODF and length distribution function (LDF), and the prediction accuracy can be further improved. Finally, the effects of the number-average fiber length and the weight-average fiber length on the mechanical properties were investigated.

An Energy-Based DG Method for Second Order Wave Equations

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ABSTRACT

We present a new method for constructing discontinuous Galerkin methods for wave equations in second order form. The weak form works directly with the Lagrangian of the system. By Noether's Theorem, given any symmetry of the Lagrangian, one can derive a conservation law on a given element. Our method is built on such conservation laws, with the weak form chosen so that the rate of change of the conserved quantity is determined by the flux through the element boundaries. These can be chosen either to exactly preserve a discretization of the conserved quantity or to dissipate it in proportion to jumps across the inter-element boundaries. If the conserved quantity is positive definite, as in the energy for typical physical systems, we can conclude that the method is stable and convergent. We have applied our construction to a variety of problems ranging from the simple scalar wave equation (Appelo and Hagstrom, SINUM, 53, 2015) to linear elasticity (Appelo and Hagstrom, CMAME, in revision). In this talk we focus on its application to the convective wave equation. Here some new features arise. First, the energy is not associated purely with time symmetry, but rather with a specific combination of space and time symmetry. Second, depending on whether the background flow projected in the direction normal to the element boundary is subsonic or supersonic, upwind fluxes must be defined in different ways. We will outline the convergence analysis of the method in this case and demonstrate optimal high-order convergence for some simple examples.

A Micromorphic Model for Strength Analysis on Carbon Nanotube Reinforced Concrete: Modeling and Experiments

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ABSTRACT

Concrete exhibits a large number of microcracks during the application of any external loads, which have a significant effect on the mechanical behavior of concrete and contribute to nonlinear behavior at low stress levels. CNTs can act as crack bridges inside concrete, making it less porous and improving its flexural strength and toughness significantly. In order to dig deeper into the mechanical properties of CNT-reinforced concrete composite, a multiscale micromorphic framework is established to simulate the phases and interface in different constitutive models, for the purpose of linking continuum behavior of CNT reinforced concrete and its microstructure. In this investigation, the geometry of RVE is considered in which the CNT and matrix are taken as elastic continua. A morphological kinematic descriptor is used to characterize the fiber-matrix bond-slip mechanism). The equilibrium equations of conventional Cauchy stress at the macroscale, as well as generalized microstress at the mesoscale, are established. A staggered algorithm is implemented to solve the coupled problem, including the additional DOFs associated with the micromorphic fields. The mixture theory is used as the methodological approach to model reinforced composites. The iterative solution procedure using the Newton–Raphson method with displacement control is employed to solve the system of equations for each incremental step. Several numerical examples are carried out to demonstrate the proposed model’s capability of representing adequately the effects of microscopic bond sliding on the overall macroscopic deformation of CNT-reinforced cement composite structures.

Adaptive Interface for the Immersed Finite Element Method

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ABSTRACT

Despite the great advantage of not having to constantly re-meshing the computational domain, one of the major challenges in the immersed methods is the resolution or the sharpness at the fluid-structure interface. When dealing with non-conformed meshes, the interaction is handled by the interpolation between meshes. As a result of the interpolation, the interface is often not sharp enough to reflect accurately the physical quantity changes or jumps such as the intrinsic material properties and resolved physical quantities between the phases such as stress and pressure. In this talk, we utilize the quad-tree mesh structure of an open-source finite element library deal.II, where the cells in the grid can be conveniently split or merged based on a locally defined criterion. We choose to use the second order derivative of the “fluid-structure interaction force” as an indicator of mesh adaption in the neighborhood of the fluid-structure interface in the background fluid grid. Upon the adaptive refinement, the interface is precisely tracked and represented during the dynamic fluid-structure interactions, yet the total number of degrees of freedom is controlled in a reasonable range without knowing the general solid location a priori. This adaptive interface is conveniently implemented in our refactored immersed finite element method (IFEM) code. Our newly developed open source, high performance IFEM code, open-IFEM, utilizes a series of open source libraries, and is published on Github. We welcome potential users to use and contribute to this open-source project.

Calibrated Growth Model for In-stent Restenosis Using Patient Data

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ABSTRACT

The in-stent restenosis is a common adverse event of vascular 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 use a growth model to simulate tissue growth and remodeling based on mechanical stimulants such as stent deployment. The growth model is calibrated based on patient data to produce binary in-stent restenosis prediction. The tissue wall shear stress is considered as the major mechanical stimulant. The multi-time scale coupling between short-term fluid-induced shear stress during the blood pulsatile flow within a cardiac cycle and long-term tissue growth is performed using the concept of small-on-large. This study provides a useful simulation approach to predict the risks of in-stent restenosis, which ultimately provides better patient care and planning.

A Rheology Model Incorporating Scale Effect for Rockfills

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ABSTRACT

Scale effect of rockfills can hardly be captured by classical constitutive models because those models are independent of scale. Based on Cosserat continuum theory, this study extended the Perzyna's viscoplastic model for describing the scale effect in the rheological behavior of rockfills. We derived the constitutive integration algorithm and the closed form of the consistent tangent modulus for this model. This model was implemented in ABAQUS by means of User Element Interface (UEL). The results of numerical simulations were compared to those typical experiments as tri-axial creep tests of soft rock, stress relaxation tests of black slate rockfill and creep tests of granite rockfill. The numerical results were in a good agreement with the experimental data so that the validity of this model was proved. We introduced parameters, such as the sphericity index, roundness index, and mean diameter of the particle, into our model, by relating the internal length with those parameters via the equation suggested by Voyiadjis. Then, we investigated the influence of particle size and shape on axial strain, deviator strain and deviator stress using this viscoplastic model. Time-dependent deformation of a typical Concrete-Faced Rockfill Dam was analyzed using FEM with this viscoplastic model as the constitutive equation of rockfills. The settlement of the dam predicted by the simulation agrees well with the result from site observation.

Effect of Phase Transition on Mechanical Properties of NIPA Hydrogel by Tensile Test

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ABSTRACT

Poly(N-isopropylacrylamide) (NIPA) hydrogel is one of the most extensively studied temperature-sensitive hydrogel, displaying a lower critical solution temperature (LCST) in aqueous solution and undergoing an abrupt thermo-reversible change in volume as the external temperature cycles around LCST (type α phase transition). Due to the lower temperature of phase transition (30°C - 35°C), the NIPA hydrogels have attracted great interest for a wide variety of applications, such as artificial organs, actuators, drug delivery, on-off switches, etc. Moreover, phase transition can also be induced by tensile force (type β phase transition) in some experimental phenomenon. However, the mechanical behaviors of NIPA hydrogel induced by two types phase transitions are still not well understood. Therefore, in this study, two types phase transitions as well as their coupling effect on mechanical properties of NIPA hydrogel are quantitatively studied from simulation and experiment. The mechanical properties of self-prepared NIPA hydrogel with LCST around 35°C under monotonic load and cyclic load using tensile test are studied with different temperatures. It is found that type β phase transition greatly influenced the mechanical properties of NIPA hydrogel during the tensile process. The maximum nominal stress and maximum stretch above the LCST are larger than those of below the LCST. We also find that the samples around LCST are easy to rupture, because of phase coexistent. The gels under type β phase transition, to some extent, behave some toughening characteristics, in particular, under cyclic load. Furthermore, the phase transition induced by tensile force is irreversible. In addition, adopting the existing theory of temperature-sensitive hydrogel, numerical simulations are carried out using parameters' value that determined by experiments. It can be found that the simulation results agreed well with the experimental results.

Simulation of Seismic Energy Dissipation in Concrete Gravity Dams Using a Smeared Crack Approach

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ABSTRACT

Abstract: Seismic energy dissipation analysis of concrete gravity dams is presented based on an improved smeared crack model. The hysteretic behavior for concrete under tension-compression reversals due to the crack closing and reopening mechanism is simulated by the proposed model. Cracked shear modulus is suggested as a function of the normal strain in the directions perpendicular to the crack plane. The conservation of fracture energy and strain-rate effect are considered at the same time. Two-dimensional seismic response analyses of koyna dam are performed to demonstrate the application of the proposed model. The influence of hysteretic behavior under tension-compression reversals on the seismic cracking and dissipation energy accumulation of concrete dams are discussed. The main novelty of the present paper is the proposed model considering the hysteretic behavior for concrete under tension-compression reversals. The effect of earthquake duration on the seismic energy dissipation of concrete dams can be taken into account by means of the proposed model, which is significant for the seismic damage assessment of concrete dams.

An Improved Staggered Iteration Scheme for the Modelling of Cohesive Zone Based Fracture by Phase Field Method

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ABSTRACT

Recently phase field model has gained popularity because of its convenience of analyzing crack initiation and propagation. In the present study a cohesive law based phase field model is implemented in the commercial finite software Abaqus with the user subroutine UEL (user defined element). The traction-separation relationship involved in the cohesive model has increased the solving difficulty of modeling significantly. Especially for the convergence issue which could result in the abortion of simulation without proper iteration algorithm. In order to improve the robustness and efficiency of the model, existing iteration algorithms are discussed in detail by using an analogical method. Based on the obtained results, a new improved iteration algorithm based on the staggered iteration scheme is proposed for the modelling of cohesive fracture. Numerical results show that both the crack path and load versus displacement curve predicted by the proposed method are in good agreement with the experimental observation and other numerical results. Furthermore, through the comparison of the iteration numbers of each incremental load between the present improved algorithm and the staggered iteration algorithm, it is proven that the proposed method is more effective for phase field modeling of cohesive fracture.

Tunable Metamaterials for Manipulating Elastic Wave through Transformation Method

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ABSTRACT

Elastic metamaterials have attracted significant interest in recent years because of their broad range of applications, including vibration isolation, wave guiding, cloaking, and focusing [1]. Practically, traditional elastic metamaterials only operate at fixed frequency ranges due to the fixed microstructure, limiting additional potential applications. To address this issue, electromagnets, shape memory effect, structural deformation, fluid-structure interaction, and piezo-shunting have been employed to achieve elastic metamaterials with tunable band gaps [2,3]. These current strategies for designing tunable locally resonant metamaterials are all based on tuning the stiffness of the resonator. The most notable shortcoming of this approach is that the high frequency effective mass density is a constant, contrary to the request of transformation method based on density regulation. The high frequency effective mass density of locally resonant metamaterials is simply determined by the mass of substrate, which can be easily tuned if the mass distribution between resonator and substrate is changeable. Here, this paper reports a type of tunable locally elastic metamaterial, which consists of several liquid or gas inclusions in a solid matrix, controlled through a pair of embedded pumps. Both band gaps and effective mass density at high frequency can be tuned by controlling the liquid distribution in the unit cell, as demonstrated through a combination of theoretical analysis, numerical simulation, and experimental testing. Finally, we point out that our method can be utilized in steering wave propagation through transformation method based on density regulation. Our study offers a new perspective to design tunable metamaterials through controlling mass distribution, providing new avenues for vibration isolation and wave guiding. Reference: [1] O.R. Bilal, A. Foehr, C. Daraio, *Adv. Mater.* 2017, 29, 1700628. [2] Z. Wang, Q. Zhang, K. Zhang, G. Hu, *Adv. Mater.* 2016, 28, 9857. [3] P. Wang, F. Casadei, S. Shan, J.C. Weaver, K. Bertoldi, *Phys. Rev. Lett.* 2014, 113, 014301.

A Multiscale Space-time Computational Framework for Fracture and Fatigue Failure Simulation

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ABSTRACT

We present a multiscale computational framework based on the coupling of time-discontinuous Galerkin (TDG) based space-time finite element method with either a two-scale damage model or Peridynamics (PD) for the purpose of fracture and fatigue failure simulation. This approach takes full advantage of the space-time FEM and its extended version (XTFEM) [1-3] in capturing multiple temporal scales, sharp gradients and discontinuities that are frequently encountered in these applications. An accelerated implementation of space-time FEM is developed to further improve its numerical efficiency. After outlining the basic framework, we first describe the integration with a two-scale models based on continuum damage mechanics. Sets of parameters for these damage models are calibrated by fatigue experiments of materials such as steel and synthetic rubber. We then present the work on the coupling of XTFEM simulation with PD simulation to capture crack initiation and propagation. To accommodate the evolving nature of the dynamic fracture, an adaptive scheme is developed so that the PD simulation is prescribed dynamically at the region near crack tip. Finally, a physics-based projection approach is introduced to realize seamless coupling between the two methods. Direct numerical simulations of high cycle fatigue over one million cycles are successfully performed with the presented framework. The results are validated through comparison with experiments and comparisons with full PD simulation of brittle fracture propagation. References: [1] 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. [2] 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. [3] S. Wada, R. Zhang, S. R. Mannava, V. K. Vasudevan, and D. Qian, "Simulation-based prediction of cyclic failure in rubbery materials using nonlinear space-time finite element method coupled with continuum damage mechanics," Finite Elements in Analysis and Design, vol. 138, pp. 21-30, 2018.

A Phase Field Model for Simulation of Crack Propagation in Anisotropic Materials and Its Application to Predict Fracture Behavior in Silicon Carbide

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ABSTRACT

Crack initiation and fracture is of utmost concern in all engineering applications. Understanding fracture is complicated by its high sensitivity to the material microstructure, with defects typically serving as locations for crack initiation. Phase field modeling has been proved to an efficient tool for simulating crack initiation and propagation in materials, and several successful fracture models have been developed for isotropic materials in the recent past. However, the anisotropic nature of most crystal lattices necessitates a model that account for anisotropic material behavior. In this presentation, we present an anisotropic phase field model that can account for the impact of material microstructure on crack initiation and propagation. First, numerical examples are shown for verification of this phase field fracture model. Then, results from molecular dynamics simulations are used to parameterize the model for SiC. Finally, the model is used to predict fracture in polycrystalline SiC.

Understanding Wrinkles and Folds in Elastic Thin Sheets via a Lattice Model

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ABSTRACT

Thin elastic sheets can undergo complicated instabilities even under simple loads, examples including wrinkles and folds of a floating thin sheets due to liquid surface tension. A very rich instability phase diagram can emerge in thin sheets with simple geometries, such as annular and rectangular strip, which is determined by the nonlinear interplay of bending energy, gravity potential, surface energy and external work. In this talk, I will show from two examples, annular wrinkles and folds in a strip, that a triangle lattice model can efficiently and robustly capture these nonlinear instability modes. For the annular wrinkling problem, we will compare numerical predictions from the lattice model with experiments, perturbation theory at the near-threshold instability, and energy methods at the far-from threshold instability. It will be shown that the lattice model are all in very good agreements with the existing experiments and theories. For the folds in a strip under compression, we will explicitly account for the geometry nonlinearity of the gravity potential and self-contact of the solid film to avoid penetration. We will validate the lattice model by comparing it with an exact solution from full nonlinear analysis before self-contact and a reduced one-dimensional rod model.

A Moving Morphable Void (MMV)-based Explicit Approach for Topology Optimization Considering Stress Constraints

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ABSTRACT

Topology optimization considering stress constraints has received ever-increasing attention in recent years for both of its academic challenges and great potential in real-world engineering applications. Traditionally, stress-constrained topology optimization problems are solved with approaches where structural geometry/topology is represented in an implicit way. This treatment, however, would lead to problems such as the existence of singular optima, the risk of low accuracy of calculated stress magnitude, and the lack of direct link between optimized results and computer-aided design/engineering (CAD/CAE) systems. With the aim of resolving the aforementioned issues in a systematic and straightforward way, a Moving Morphable Void (MMV)-based approach is proposed in the present study. Compared with existing approaches, the distinctive advantage of the proposed approach is that the structural geometry/topology is described in a completely explicit way. This feature provides the possibility of obtaining optimized designs with crisp and explicitly parameterized boundaries using much fewer numbers of degrees of freedom for finite element analysis and design variables for optimization, respectively. Several numerical examples provided demonstrate the effectiveness and advantages of the proposed approach.

Infrared Grating Thermal Wave Imaging for Detection of Damage in Thin Film System

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ABSTRACT

Interfacial damage significantly influences the reliability of thin film. For a very thin multi-layer film, how to accurately locate the damage is a big challenge. We introduced a new infrared grating thermal wave imaging to detect the damage in the thin film. The fundamental theoretical analysis of this approach will be presented. The effectiveness of this approach is validated by numerical simulation and experiment. The new approach is of high accuracy to locate the position of damage in principle.

A Contact Analysis Study for Rough Surfaces Considering Sliding-impact Behavior

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ABSTRACT

Most of the typical coupling sliding-impact behavior are caused by thermal-solid-liquid complex operational environment. It may result in contact interface damage and even catastrophic consequences. The key point to solve this problem is to reveal the contact damage mechanism of sliding-impact behavior which happens on the typical contact interface. The actual damage can be caused by permanent deformation of two rough surfaces. This paper presents a theoretical study on the contact deformation process based on the elastoplastic deformation theory and the fractal theory. It can reveal the micro elastic-plastic contact mechanism and the statistical characteristics of macro contact with in consideration of the coupling sliding/impact behavior. Firstly, a revised W-M fractal contact model under the fixed load has been established. Then, the influence of impact on the contact variables of the revised W-M fractal contact model, such as the mean contact pressure, the contact area and the contact load are further analyzed by changing the magnitude of the impact energy and fixed contact loads. In addition, the equivalent contact load of uncertain time-varying impact under different contact mechanisms is also included.

Initial Solution Estimation for One-step Inverse Isogeometric Analysis in Sheet Metal Stamping

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ABSTRACT

Recently, Isogeometric Analysis (IGA) based on incremental methods for simulating the stamping process has been researched. To the best of our knowledge, however, few studies have combined IGA and One-step inverse approach which is based on total deformation theory of plasticity. A key step for One-step inverse IGA is to estimate a good initial solution. Traditional mesh-based initial solution algorithms for One-step inverse approach are not suitable for One-step inverse NURBS-based IGA. In this paper, we presented a method which can rapidly unfold the undevelopable NURBS surface onto a planar domain and obtain a good initial solution estimation for One-step inverse IGA. The key idea of the presented method is unfolding the control net of a NURBS surface for isogeometric analysis by energy-based initial solution estimation algorithm. In addition, we developed a "cutting-stitching" algorithm which can separate a complex control net into several parts with simple shapes. Numerical examples illustrate the initial solutions using the presented method are approaching the final results by One-step inverse finite element method. This implies that the iterative steps and computational time of One-step inverse IGA will be reduced significantly compared with that of One-step inverse finite element method.

CFD Simulation of Piston-cylinder Jet Flows in Marine Propulsion

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ABSTRACT

As a result of natural selection, fast moving marine animals choose impulsive modes to swim. Examples are: a squid generates an impulsive jet for thrust through its body muscle contraction, and a fish, through a control of the flapping of its caudal fin, is able to create an impulsive jet with a feature of thrust vectoring. A great amount of experimental work has been carried out to study impulsive jets and the associated vortex rings through the starting flows generated from a piston-cylinder apparatus. The research showed the efficiency advantage of an impulsive jet for propulsion lies in the utilization of the largest possible isolated vortex ring an impulsive jet can generate before its pinch-off from the trailing jet. With growing interests for a practical use of impulsive jet in marine propulsion, numerical simulation capabilities for impulsive jet flows become of obvious importance. Numerical simulation capabilities are challenged by the highly transient and vortical nature in the impulsive jet flows. Most of studies in the numerical simulations for the impulsive jet flows, especially the starting flows from a piston-cylinder apparatus, were for low Reynolds numbers in the scale of marine animals. Few numerical simulations were found for impulsive jetting into a background flow. CFD solver based on OpenFOAM was applied to simulate the starting flows by a piston-cylinder apparatus at Reynolds numbers from low to high covering marine animals and practical marine propulsors, and with various background flows. Numerical aspects such as numerical schemes, grid sensitivity and convergence quality in terms of the accuracy in capturing the flow vortical structures in the transient flow fields were studied. The numerical simulations were first validated and verified against those from the experimental and numerical studies found in the literature in the low Reynolds number range with and without background flows. The simulation tool was then applied to the predictions of the impulsive jet flows in the high Reynolds number range in practical marine propulsion with background flows.

Winkle Patterns on Torus

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ABSTRACT

We investigate wrinkle patterns in a torus tripe-layer, where a thin outer layer is under expansion to drive the formation and evolution of wrinkles and an inner core has a tunable modulus to adjust the confinement of global expansion of the torus. We show from large-scale finite element simulations that hexagonal patterns will form at strong confinements (i.e. a stiff core) and strip wrinkles will develop at weak confinements (i.e. a soft core). Hexagons and strips can co-exist to form hybrid patterns at an intermediate confinement. As the outer layer further expands, strip and hexagon patterns will evolve into Zigzag and segment labyrinth, respectively. In addition, we observe strip wrinkles tend to initiate from the inner surface of the torus while hexagon wrinkles start from the outer surface. We further quantitatively analyze the topological defect distribution for a representative hexagonal pattern.

Numerical Modeling and Experimental Validation of Hyper Velocity Impact of a Multi-Layer Fabric Coated Aluminum Plate

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ABSTRACT

Due to their excellent impact-resistance, anti-fatigue and energy absorption capacity, fabrics and flexible composites are frequently used in protective structures to enhance their protective capacity. For example, a multi-layer fabric coated aluminum plate is usually used in the hard-upper torso of a space suit to protect astronauts from getting hurt by space dust, where the multi-layer fabric consists of an outer-layer fabric, a multi-layer insulation (MLI) layer and a liner layer. In this work, the protective performance of the multi-layer fabric coated aluminum plate is investigated both experimentally and numerically. To provide benchmarks for validating our numerical method, thirteen hyper velocity impact tests with different impact velocities (maximum velocity is 6.19km/s) and projectile diameters have been conducted. Due to the limitations of test equipment capacity, the hypervelocity impact tests with impact velocity higher than 6.2km/s are hard to be conducted. Therefore, a material point method (MPM) model is established for the multi-layer fabric coated aluminum plate and validated/corrected using our test results for impact velocity less than 6.2km/s. An equivalent laminated plate model of the MLI layer, which is composed of aluminized films separated by gauzes, is established to avoid discretizing its each single-layer which is too thin. A ballistic limit equation is established for the multi-layer fabric coated aluminum plate for space suit design by using the hyper velocity test results for impact velocity less than 6.2km/s and the MPM simulation results for impact velocity greater than 6.2 km/s. It shows that the critical diameter obtained by the validated MPM model for impact velocity less than 6.2km/s agrees well to the established ballistic limit equation, although which is established based on the test results for these velocity range. The corrected MPM model and the ballistic limit equation developed for the multi-layer fabric coated aluminum plate provide an effective tool for the space suit design.

The Nonlinear Controlling Effectiveness and Failure Mechanism of the MSCS

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ABSTRACT

Mega-sub controlled structure (MSCS) is a new form of super tall buildings which is installed dissipation dampers to consume dynamic energy associated with excellent earthquake-resistant capability, and is stronger nonlinearity. However, as the nonlinear controlling effectiveness and failure mechanism of a practical MSCSS is different from the traditional mega sub structure (MSS), it is necessary to further investigate its nonlinear controlling effectiveness and failure mechanism. This paper focuses on the Mega-Sub Controlled Structure Systems (MSCSS) performances and characteristics regarding the new control principle contained in MSCSS subjected to strong earthquake excitations. The adopted control scheme consists of modulated sub-structures where the control action is achieved by viscous dampers and sub-structure own configuration. The elastic-plastic time history analysis under severe earthquake excitation is analyzed base on the Finite Element Analysis Method (FEAM), and some comparison results are also given in this paper. The result shows that the MSCSS systems can remarkably reduce vibrations effects more than the mega-sub structure (MSS). The study illustrates that the improved MSCSS presents good seismic resistance ability even at 1.2g and can absorb seismic energy in the structure, thus imply that structural members cross section can be reduce and achieve to good economic characteristics. Furthermore, the elasto-plastic analysis demonstrates that the MSCSS is accurate enough regarding international building evaluation and design codes. This paper also shows that the elasto-plastic dynamic analysis method is a reasonable and reliable analysis method for structures subjected to strong earthquake excitations and that the computed results are more precise. Keywords: controlling effectiveness, Elasto-plastic dynamic analysis, Mega-Sub Controlled Structure, Plastic hinge pattern.

Multi-scale Concurrent Topology Optimization for Macrostructures with Multi-patch Microstructures

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ABSTRACT

Due to the capability of the fully exploring materials distribution at the macroscopic and materials configuration at the microscopic, the multi-scale concurrent topology optimization can obtain more excellent structural performance than the monoscale design by either sole macrostructures optimization or materials design. The intensive computational cost on material microstructures varying from point to point at the macroscopic scale is the main restriction on applications of the multi-scale concurrent topology optimization. This work develops a novel multi-scale concurrent design framework for topology optimization of material and structure to obtain the most excellent structural performance with a given material usage and an affordable computation cost. In this framework, the macrostructure consists of multiple kinds of material microstructures. Firstly, an ordered SIMP interpolation method, which is efficient to solve multi-material topology optimization problems without introducing any new variables, is presented to generate an optimized structure layout with the predetermined element density at macro scale. Then, all macro elements with the same density are considered to have the same microstructural configuration at micro scale. A parametric level set method is applied to the evolution of the shape and topology of the microstructures, whose effective properties are evaluated by the numerical homogenization approach. The kinematical connective constraint approach is employed to guarantee the connectivity of neighboring microstructures. In this way, the proposed method can simultaneously generate optimized macro material distribution patterns as well as optimized material microstructural configurations. Finally, some reasonable design solutions of the macrostructure and several material microstructures are obtained under the significantly reduced computation cost.

A New Design of Joint-bonded Triangular Cell Lattice Metamaterial with High Stiffness and Unbounded Thermal Expansion

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ABSTRACT

Triangular cell lattice metamaterials composed of bi-layer curved rib elements (called the Lehman-Lakes lattice) possess unbounded thermal expansion, high stiffness and shear impossibility of thermal buckling, which are highly desirable in many engineering structural application subjected to large fluctuations in temperature. However, the requirement of such lattice metamaterial must be pin-connected joints. The fabrication complexity makes them less than ideal for consideration especially on microstructural scales. In this study, a newly designed bi-layer curved rib element that the layer one is partially covered with layer two is proposed, which can assemble the joint-bonded lattice metamaterials with any cell topologies. As an example, the joint-bonded triangular cell lattice metamaterial (JTCLM) that is presented, which can achieve high stiffness and the desired CETs from infinite small (negative) to infinite great (positive) by intentionally adjusting the used materials and geometric parameters of rib elements. The thermomechanical properties of JTCLM are given by the closed-form analytical solution. The validity of the analytical models is illustrated and proved by the numerical simulations. Furthermore, the used materials are considered to be invar and steel, two design targets of JTCLM are obtained by optimizing the geometric parameters of rib element. One target is the stiffest JTCLM with the highest tunability for realizing large positive or negative CTEs, and the other is the stiffest JTCLM with zero CTE. Compared with the Lehman-Lakes lattice, the JTCLM with the same large positive or negative CTEs can achieve more than four times stiffness improvement; the JTCLM with zero CTE has more than 56% improvement in stiffness and simultaneously have a 34% reduction in weight. The better manufacturability and multifunctional properties of the new proposed JTCLM display a great potential for a wide range of applications.

Study on a Delamination Control Method for Composite Materials Based on Shape Memory Alloy

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ABSTRACT

Carbon fiber reinforced composite laminates have been widely used in the field of aerospace for the high specific strength and specific stiffness. However, the laminated characteristics of resin-based composites cause relatively low interlaminar mechanical properties, and the large area delamination caused by low-velocity impact would further lead to the deterioration of structural buckling characteristics. In order to reduce the damage under low-velocity impact and control the delamination area of resin-based composites, a new damage control method of embedding shape memory alloy (SMA) into composite material was proposed in this study. And based on the pseudo-elastic property of SMA, the impact damage characterization method of SMA reinforced resin-based composites laminates were explored. The numerical model of SMA reinforced resin-composites include three different parts, SMA wire, laminates layer and interface between layers. In this paper, a macroscopic thermodynamic constitutive model of SMA was studied based on previous research on phenomenological constitutive model, and this material model was used to describe the deformation process of SMA wire which combined into classical laminates numerical model. Here, to describe characteristics of interface damage between layers, the cohesive method was applied. In order to preliminarily calibrate the material parameters, the tensile test of SMA reinforced resin-based composites laminates was carried out, some parameters of material are determined by comparing the numerical model with the experimental results. After that, a numerical model of SMA reinforced resin-based composite laminates under low-velocity impact loading was established based on above method. According to the numerical results, the phenomena of delamination control for composite materials by SMA was analysed. Furthermore, the damage mechanism of SMA reinforced resin-based composites laminates was summarized.

Sensitivity of Topology Features in Stress Tensor Fields over Mesh Refinement

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ABSTRACT

Hexahedral meshes are important in tensor field visualization, such as the stress and strain tensors obtained from finite element modeling of solid mechanics. In this talk, we discuss features in 3D tensor fields that are sensitive to mesh refinement and how to classify features that are topology artifacts that are due to improper meshes.

Stress- and Temperature-Induced Phase Transformation in Architecture Materials

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ABSTRACT

Phase transforming cellular materials are architected materials whose unit cells have multiple stable configurations. If designed correctly, these materials can absorb energy by allowing controlled snap-through mechanisms as the cells transform between different stable configurations. Most previous works on architecture materials with snap-through mechanisms focused on material behavior when the material is loaded in one direction. Mostly because, most of the designs were limited to 1D behavior. In this work, we propose a new family of 2D structures defined by the number of axis of symmetry through a combined analytical, computational and experimental approach. This includes a new family of cellular architectures that employ cylindrical shell elements dissipate energy by triggering local snap-through instabilities. Physical samples were manufactured and tested in loading and unloading cycles. Ancillary analytical and computational analysis guided the design and help understand the different mechanisms acting in the system for energy dissipation. Our mechanical tests have shown key similarities in deformation modes with the simulations, and verified that there is significant energy dissipation due to snapping instabilities as expected. We also look at the application of these mechanisms to the design of temperature-induced phase transformation taking into advantage design and combination of materials to produce shape memory and actuation capabilities.

Numerical and Experimental Studies on Microstructures and Mechanical Properties in Friction Stir Additive Manufacturing

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ABSTRACT

Friction Stir Additive Manufacturing (FSAM) is a new developed technology based on friction stir welding. The plates can be joined together in a solid state by the friction from the rotating tool. In FSAM, recrystallization occurs and then the grains can be coarsened by the following temperature variations. The recrystallization and grain coarsening can be simulated by Monte Carlo method. The precipitate evolution can be also investigated. The pinning effect of precipitates is studied. The mechanical property can be divided into different components including the contributions from dislocation density, from the crystal plasticity for pure aluminum, from solid solutions, and from the precipitates. Each component is calculated and results show that the contribution from the precipitates is the main factor for the determination of the final mechanical property of aluminum in FSAM. Experiments are performed to validate the final predicted mechanical property. Acknowledgements: This study is funded by the National Natural Science Foundation of China (No. 11572074) and the Fundamental Research Funds for the Central Universities.

Optimized Design of 3D Printed Trachea for Cancer Patients

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ABSTRACT

The tracheal stent is widely used in the treatment of airway malformation may be caused by stenosis, malacia, traumatic injury, and external compression from cancer. However, these stents present some critical problems which include the growth of obstructed granulation tissue inside of trachea, and frequent migration of the stent. Improvements of tracheal stent design have been primarily focused on using new stent materials (e.g., metal, silicone, carbon nano-composite, shape memory materials). Customized patient-specific designs to ease obstructions or alleviate compressions and/or closing of trachea openings have not been explored in a systematic way. In this research, we take a systematic approach to study the airflow behavior in trachea airway due to obstruction focused for cancer patients. Using patient-specific computed tomography (CT) images, we propose an approach to solve the post-stent implantation problem and find the optimized design. Parametric studies on the length of branches and the angle between branches in the silicone stent, the flow rate, pressure drop were carried out. Computational fluid dynamics (CFD) approach was used to evaluate the performance of design with these variable parameters. Different obstructions pattern in the stent were also analyzed using CFD to imitate the shape change caused by the external compression from cancer around the trachea. Additionally, the geometry of trachea from CT images was modified with obstructions to simulate how external compression from cancer can disturb airflow behavior.

3D Crystal-Plastic Particle-in-Cell Simulation of Open-Cell Metal Foam

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ABSTRACT

Open-cell metallic foams are hierarchical structural-material systems that have applications as light-weight impact absorbers, noise insulators, and heat sinks, to name a few. Their hierarchical structure includes the grain scale, the scale of individual ligaments, and the topological scale of the foam. Many researchers have related the bulk mechanical properties of these cellular solids to the nominal density and to other metrics at the topological scale. Far fewer studies have investigated the dependence of bulk and local mechanical response on grain-scale structure of the foam. This talk will describe a high-fidelity numerical framework that captures the deformation mechanisms across multiple length scales in open-cell aluminum foam. Due to large deformations at the ligament scale in the foam during compressive loading, the finite element method tends to produce divergent results as Lagrangian meshes become extremely distorted and entangled. Utilizing the material point method (MPM), the framework presented here accommodates large deformations in the foam, since the background grid is incrementally reset during the simulation while state variables are stored at the MPM particles. Convected-particle tetrahedral domain integration (CPTI) is used, which enables a conformal representation of the ligament morphologies and grain boundaries within each ligament. To accurately predict the local, micromechanical deformations at the grain scale, a crystal-plasticity constitutive model has been incorporated into the MPM driver. The crystal-plastic material point-based (CPMPM) framework is demonstrated to simulate the deformation of foam at a mesoscale and enables simulation of the compressive behavior all the way to the foam-densification regimes. A parallel effort involves multi-scale experiments to map 3D grain structure in a real sample of open-cell aluminum foam using far-field high-energy X-ray diffraction microscopy (HEDM). The measured grain-scale data is used in the subsequent virtual reconstruction of foam geometry and generation of CPMPM models. Four cases with different grain instantiations (one measured and three synthetic) are investigated to quantitatively analyze the size effects of ligaments on the mechanical behaviors of open-cell metallic foam using the CPMPM framework. The simulation results provide insight into the correlation of local and global mechanical properties with foam microstructural features. With this new insight, well-established microstructure-based design criteria will facilitate performance-based optimization of open-cell metallic foams.

Experimental Study and State-based Peridynamic Simulation of Crack/Crack System Propagation and Coalescence in Pre-cracked Sandstone Disks under Compressive Loading

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ABSTRACT

Abstract The rock is a natural formation of mineral aggregates, generally contains different scale voids, cracks, damage and other defects. In this work, crack/crack system propagation and coalescence in pre-cracked Brazilian disks are studied by experiment and numerical simulation. Firstly, in the experiment, sandstone disks with different single pre-cracked angles and pre-cracked crack system are under compressive line loading. Secondly, most of the current numerical analysis methods must satisfy the continuity conditions in order to solve the space differential equation, the traditional numerical methods of continuum mechanics cannot accurately describe the progressive failure process of rock complex damage accumulation, macro crack initiation and crack propagation. State-based Peridynamic model is employed to simulate crack/crack system propagation and coalescence in pre-cracked sandstone disks. The state-based Peridynamic model describes a material point in a continuum interacts directly with other neighborhood material points across a finite distance. Furthermore, compared the experimental results with numerical simulation results, it is found that the numerical results by state-based Peridynamic theory are in good agreement with the experimental results. The state-based Peridynamic model has natural advantages in analyzing crack propagation and coalescence problems. Keywords Rock mechanics; Experimental study; Numerical simulation; Peridynamic; Crack propagation

A Coupled Peridynamics-Immersed Boundary-Lattice Boltzmann Scheme for Fluid-Structure Interaction Problems

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ABSTRACT

Fluid-structure interaction is a long-standing challenging problem in engineering due to complex behaviors of solids and fluids. Thus a widely extensible computational method is emerging. In this study, we provide a general computational framework aiming at solving fluid-structure interaction problems in complex media. This scheme utilizes a nonordinary state-based peridynamics model for solid deformation and the lattice Boltzmann method for fluid flow. To avoid tracking the fraction of different phases in large deformation and fracture process of the solid, we employ a modified immersed boundary method. The numerical method is compared with analytical solutions to demonstrate convergence. It is worth noting that the peridynamics model is solved by meshless method and the lattice Boltzmann method is based on a structured mesh. So, the influence of different discretization parameters is studied in the numerical examples. This scheme is applicable to a wide range of materials and fluids, including dynamic fracture in hydraulic fracturing process. Numerical results of hydraulic fracturing simulation is shown, which is in general agreement with literature and experiments.

Bubble Assemblies in Ternary Systems with Long Range Interaction

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ABSTRACT

A nonlocal diffuse interface model, based on the Nakazawa-Ohta density functional theory for triblock copolymers, is used to study bubble assemblies in ternary systems. The model has three parameters weighing three types of long range interaction and two parameters that fix the total area of each constituent. As the parameters vary, a large number of morphological phases appear as stable stationary states. One open question related to the polarity direction of double bubble assemblies is answered numerically. Moreover, it is shown that the average size of bubbles in a single bubble assembly depends on the sum of the minority constituent areas and the long range interaction coefficients. One further identifies the ranges for area fractions and the long range interaction coefficients for double bubble assemblies.

The Application of Hybrid Stress-function Method in Piezoelectric Materials

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ABSTRACT

The finite element method (FEM) has been widely used as one of the most important tools to engineering and scientific analysis. However, FEM has been suffered from mesh distortion. Recently, a novel finite element method is developed named as hybrid stress-function (HS-F) method. The resulting plane element is immune to mesh distortion and possesses excellent performance even when the quadrilateral element is degenerated into a triangular or concave one. By applying the fundamental analytical solutions of stress field to FEM, the HS-F opens a new way to develop shape-free finite element models. In this paper, we generalize the high-performance HS-F method to piezoelectric materials. Firstly, a systematic approach to determine the polynomial stress function for piezoelectric plane problems is presented based on Lekhnitskii's anisotropic elastic theory and Sosa's analytical method. Secondly, by introducing the first 23 generalized stress functions, a new HGSE-23 element is constructed based on the principle of minimum mechanical enthalpy. Finally, several numerical examples of classic problems are given to test the new element. The results show that the element inherits the advantages of HS-F method. It is a new mesh-free method for analysis of piezoelectric materials and also has very high accuracy. Moreover, the procedure may provide a guidance to develop other high-performance elements for coupling fields based on HS-F method.

Investigation of Solidification Conditions in Electron Beam Melting Using Computational thermal-Fluid Dynamics Simulation

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ABSTRACT

Electron beam melting (EBM), an additive manufacturing (AM) technology, is capable of fabricating dense metallic components using a high-intensity electron beam to melt powder layer by layer. Compared with laser powder-bed fusion process, EBM has high power density, fast melting rate and low residual stresses [1, 2]. For wide applications of EBM-built alloys, flexible control of not only the geometry but also the microstructures are highly demanded. The grains grow epitaxially from the base-metal in nature, easily producing columnar grains. For grain structure control, solidification conditions ((i) constitutional undercooling, (ii) convective fluid flow and (iii) molten pool geometry) are worthy of attention. The interaction between high-energy beam and material causes strong fluid flow in the molten pool and affect final grain morphology. In this study, the computational thermal-fluid dynamics (CtFD) simulation was applied to analyze the heat transfer, fluid flow and resultant solidification conditions, and then to inspect the effects of solidification conditions on grain morphology. CtFD simulation, which is based on a finite-difference methods (FDM), can track the front of the molten metal by the volume-of-fluid (VOF) method and predict temperature field and fluid flow. The proof-of-concept experiments were carried out in EBM apparatus using biomedical Co-Cr-Mo (CCM) alloy by way of example. The local solidification conditions, including temperature gradient (G), solidification rate (R) and fluid velocity (U) at the solidification front, were extracted from simulation results. Through the analysis of the simulated data and the experimental result, the solidification behavior within dynamic molten pool was studied. The study revealed the profound influence of fluid flow rather than G and R on grain morphology. Higher fluid velocity (U) at solidification front was found to be a quite important factor to promote CET in EBM process of CCM alloy. In addition, greatly variable normal direction of solidification front also contributes to the formation of equiaxed grains. This study also showed great prospect of controlling grain structure with the aid of quantitatively numerical simulation, which will contribute to the development of EBM-built alloys with desired property. References [1] SS Gajapathi, SK Mitra, PF Mendez. *Int. J. Heat Mass Transfer*, 54.25 (2011): 5545-5553. [2] Sochalski-Kolbus, L. M., et al. *Metall. Mater. Trans. A*, 46.3 (2015): 1419-1432.

Application of Surface Nanocrystallization in the Energy Absorption Devices

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ABSTRACT

The increasing of motor vehicles leads to frequent occurrence of traffic accidents. To improve the safety performance of automobiles, enhancing the buffering effect of the energy absorption devices during the collision accidents has become a key issue in the automobile manufacturing industry. The thin-walled structure is the most extensively used fundamental component in the energy absorption devices, which buckles easily under axial impact and absorbs a large amount of energy. Experimental results show that the geometric parameters and material properties have significant influence on the energy absorption capacity. In other words, the high-order buckling modes of the thin-walled structure can be induced by optimized parameters, which could directly improve the energy absorption effect. At present, classical design of energy absorption devices, e.g., changing external configuration of the overall structure, adding adjunctive structures to the main body, usually increases the processing difficulty and manufacturing costs. Therefore, there is a great demand for developing a high energy absorption device without any modification of the configuration of the fundamental component. A novel surface nanocrystallization technology is an emerging technology to enhance the mechanical properties of metal material. By using the nanocrystallization technology, the local material properties of thin-walled structures are strengthened and the nanocrystallization layouts are designed easily. Thus, it provides a simple way to induce the high-order buckling modes of the thin-walled structures under impact loads. In the present study, an accurate simulation method is proposed to analyze and optimize the local nanocrystallization energy absorption devices. Firstly, on this basis of the theoretical equations, the dynamic analysis algorithm for the local nanocrystallization energy absorption devices is developed under the framework of ANSYS LS-DANA. The produce of the energy absorption is accurately predicted by the proposed algorithm. Secondly, the local nanocrystallization layouts and geometric parameters are optimized by using a structural optimization theory. The relation between the buckling mode and the key influencing factors are obtained. Compared with the thin-walled structures without nanocrystallization, the treated ones show higher energy absorption capacity and stability. It provides a new technique of designing and manufacturing such energy absorption devices for the automobiles during the collision accidents. The present study not only promotes the development in energy absorption design but also provides guidance to the practical engineering manufacturing in various industries.

Multi-scale Finite Element Modeling on the Impact Behavior of Triaxially Braided Composites

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ABSTRACT

Carbon fiber reinforced textile/braided composite now has gradually been used in aerospace and automotive structures to defend the external impact load due to its outstanding impact resistance. For instance, the two-dimensional tri-axially braided composite (2DTBC) is introduced to fabricate engine fan case structure, which exhibits excellent damage tolerance and reduces significantly the weight of the aero-engine. Design and optimization of large-scale structures, such as the fan blade and containment casing of aero engine, is a formidable and costly task. Fortunately, finite element simulation approach has been validated for its capability in predicting the failure behavior and mechanical performance of braided composite. In addition, previous studies suggest that accurate determination of basic mechanical properties are very essential for the proper implementation of material models in impact simulations. Thus, in this work, a multi-scale method is proposed to investigate the impact response of 2DTBC. Firstly, a micromechanical model is used to obtain the properties of fiber tows which are intertwined to form the layer of 2DTBC, based on the properties of fiber and matrix extracted from literatures. Then, a validated meso-scale finite element (FE) model is adopted to simulate the failure behavior of the braided composites under different load conditions, taking into consideration the realistic test boundary conditions. Finally, an enhanced macro-scale subcell model for a six-layer braided composite plate is developed to study the impact behavior of the 2DTBC. The homogenized material properties of the subcell model is acquired by using the volume averaging method from the effective stress-strain responses of the subcell elements for the representative unit cell. The presented modeling framework presents a new tool for impact simulation of textile composites and shows advantages in capturing the failure initiation and progression during an impact load. The impact simulation results compare well with the experimental results and provide insights on the impact failure characters of this material.

Generalized Variational Principles for Fully Coupled Thermo-Chemo-Mechanical System Based on Continuum Thermodynamics

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Key words: Generalized Variational Principle, Functional, Multi-Field Coupling, Chemical Reaction, Continuum Thermodynamics

Abstract: Multi-scale and multi-physics coupling governs many complex engineering problems. Such issues with chemical or electrochemical reactions are essential for many industrial applications, such as energy storage and conversion technologies. Discussions regarding thermo-chemo-mechanical coupled problems have drawn great attention in recent years. Our previous research substantiates that the reaction extent can be treated as an internal variable for modeling multi-physics problems by means of continuum mechanics. However, few efforts have been devoted to develop variational principles and associated numerical modeling technologies of this kind of problems. Herein, two complementary generalized variational principles for fully coupled thermo-chemo-mechanical problems are established. The equivalence between the proposed generalized variational principles and the partial differential equations governing the fully coupled thermo-chemo-mechanical problems is then demonstrated. The analogy of different physical essences are discussed, which reveals the intrinsic relationship between different fields. Introducing proper preconditions simplifies corresponding variational principles to be valid for single field problems, two-field coupled or half coupled problems. Some remarkable simplifications of present theory are obtained. These simplifications corroborate former studies, indicating that all existed theories share the same theoretical basis. This work may provide a way for numerical simulating multi-physics problems, for which some numerical validations are given.

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Nomenclature

U	=Internal energy(= $E + \Phi$) / (J)	Φ	=Dissipative potential energy / (J)
E	=Free internal energy / (J)	Ψ	=Dissipative potential density / (J/m ³)
e^r	=Free internal energy density / (J/m ³)	ϕ	=Dissipative power density / (W/m ³)
\mathbf{u}	=Displacement / (m)	$\boldsymbol{\varepsilon}$	=Total strain / (-)
$\boldsymbol{\varepsilon}^r$	=Thermodynamic reversible strain / (-)	$\boldsymbol{\sigma}$	=Stress / (Pa)
$\boldsymbol{\varepsilon}^i$	=Irreversible strain / (-)	\mathbf{f}	=Body force / (N)
η^r	=Reversible entropy per unit volume / (J/K/m ³)	T	=Temperature / (K)
q	=Heat flux density / (J/m ² /s)	q^r	=Thermal dissipative intensity / (K/m)
c_α	=Number of moleculars of α influx per unit volume / (mol/m ³)	μ_α	=Chemical potential of α / (J/mol)
m_α	=Mass flux of α / (mol/m ² /s)	μ_α^μ	=Diffusion dissipative intensity of α / (J/mol/m)
$\ell^{(\gamma)}$	=Extent of reaction γ / (mol/m ³)	$A^{(\gamma)}$	=Chemical affinity / (J/mol)
r_α	=Source density of α / (mol/m ³)	$\nu_\alpha^{(\gamma)}$	=Stoichiometric coefficient of α in reaction γ / (-)
W	=Work done by external forces / (J)	\mathbf{n}	=Unit vector normal to boundary
$\bar{\mathbf{u}}$	=Prescribed boundary displacement / (m)	$\bar{\mathbf{T}}$	=Prescribed boundary force / (N/m ³)
\bar{J}_α^m	=Prescribed boundary mass flux of α / (mol/m ² /s)	$\bar{\mu}_\alpha$	=Prescribed boundary chemical potential of α / (J/mol)
\bar{q}	=Prescribed boundary modified heat flux / (J/K/m ² /s)	\bar{T}	=Prescribed boundary temperature / (K)

Subscripts/Superscripts

*	=Complementary part	q	=Related to heat conduction
r	=Thermodynamic reversible	i	=Irreversible (dissipative)
α	=Chemical species α	γ	= γ th reaction
N	= N th internal variable	m	=Related to mass diffusion

For convenience, we assume Einstein's summation convention for subscribe/superscript α and γ herein.

1 INTRODUCTION

The strong coupling of various physical quantities can be found in advanced functional materials^[1, 2], energy storage and conversion devices^[3, 4], natural porous media^[5-7], natural fiber reinforced composites^[8-10] and biological tissues^[11]. For example, gels or polyelectrolytes have typical coupling performances such that ion transportation and electrochemical reaction take place simultaneously with hyperelastic responses^[12].

Great efforts have been devoted to theoretical studies on such multi-field coupling problems in the past decades. Based on thermodynamics for mechano-chemistry^[13] and poroelasticity^[14], Rice

and Cleary^[15] solved some basic stress-diffusion problems. With more physical phenomena involved, such as temperature effect, chemical reaction and electrical response, some phenomenological models have been developed^[16-19]. In order to develop an efficient numerical method for multidisciplinary simulation, variational principles for multi-field problems attracted great research interests. Luo^[20, 21] derived generalized variational principles for thermo-mechanical and electro-mechanical coupling problems. Yang and Qin^[22] proposed a variational principle and corresponding finite element formulation of coupled thermo-electro- chemo-mechanical problems. Hu and Shen^[23] obtained a series of quasi variational principles for thermal-mechanical- chemical coupling problems by using different forms of free energy and constitutive equations. Recently, Zhang and Zhong^[24] developed a fully coupled theoretical framework for chemically active and deformable solids with mass diffusion and heat conduction, treating reaction extent as an independent variable so that the contributions of chemical reaction can be distinguished from those of species diffusion.

Generalized variational principles of Hu-Washizu type and Hellinger-Reissner type are direct theoretical basis of constructing mixed finite element method which can avoid some numerically ill-posed issues in conventional finite element method. For multi-field problems, such generalized variational principle has never been reported yet. Therefore, the main purpose of this work is to construct a suitable generalized variational principle for fully coupled thermo-chemo-mechanical problems based on the theoretical framework of Zhang and Zhong^[24], and to show the capability of the framework through examples numerically implemented.

The present work is organized as follows. First, basic equations for fully coupled multi-field problems are discussed in Section 2. Then the generalized variational principles of potential energy type and complementary energy type are established and demonstrated respectively. Section 3 is devoted to clarify the consistency with those in literature through a simplified version of proposed generalized variational principle. In Section 4, a numerical example of a reaction-diffusion process reveals the progress in present approach. Results are shown in Section 4 as well.

2 THEORETICAL MODEL

On the basis of previous studies, a thermodynamic framework considering chemical extent as an independent internal state variable was established in Ref.[24-26]. This framework governs typical thermo-chemo-mechanical coupling problems. Consider a macroscopically homogeneous body B made of a chemically active medium (a host solid with absorbed chemical species) and bounded by surface S. With deformation, mass diffusion, heat conduction and chemical reaction considered, after slight adjustment governing equations can be expressed as follows:

First constitutive equations (state equations)

$$\boldsymbol{\sigma} = \frac{\partial e^r}{\partial \boldsymbol{\varepsilon}^r} \quad T = \frac{\partial e^r}{\partial \eta^r} \quad \mu_\alpha = \frac{\partial e^r}{\partial c_\alpha} \quad A^{(\nu)} = -\frac{\partial e^r}{\partial \ell^{(\nu)}} \quad (1)$$

Second constitutive equations (evolving equations)

$$\dot{\boldsymbol{\varepsilon}}^i = \frac{\partial \phi^*}{\partial \boldsymbol{\sigma}} \quad \dot{q} = \frac{\partial \phi^*}{\partial T} \quad \dot{m}_\alpha = \frac{\partial \phi^*}{\partial \mu_\alpha} \quad \dot{\ell}^{(\nu)} = \frac{\partial \phi^*}{\partial A^{(\nu)}} \quad (2)$$

Gradient equations

$$\frac{1}{2}(\nabla \mathbf{u} + \mathbf{u} \nabla) = \boldsymbol{\varepsilon}^r + \boldsymbol{\varepsilon}^i \quad \overset{T}{q} + \nabla T = 0 \quad \overset{\mu}{\alpha} + \nabla \mu_\alpha = 0 \quad (3)$$

Balance equations

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = 0 \quad \dot{\eta}^r + \nabla \cdot \overset{T}{q} = 0 \quad \dot{c}_\alpha + \nabla \cdot \overset{m}{\alpha} = 0 \quad (4)$$

while boundary conditions are listed as follows:

Dirichlet type boundary conditions

$$\mathbf{u} = \bar{\mathbf{u}} \quad (\text{on } \partial\Omega_u) \quad T = \bar{T} \quad (\text{on } \partial\Omega_T) \quad \mu_\alpha = \bar{\mu}_\alpha \quad (\text{on } \partial\Omega_{\mu_\alpha}) \quad (5)$$

Neumann type boundary conditions

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{T}} \quad (\text{on } \partial\Omega_\sigma) \quad \overset{q}{q} \cdot \mathbf{n} = \bar{J}_q \quad (\text{on } \partial\Omega_q) \quad \overset{m}{\alpha} \cdot \mathbf{n} = \bar{J}_\alpha^m \quad (\text{on } \partial\Omega_\alpha^m) \quad (6)$$

where Ω is the control volume of body B with the outward unit vector \mathbf{n} normal to its boundary $\partial\Omega$, $\partial\Omega = \partial\Omega_u \cup \partial\Omega_\sigma = \partial\Omega_q \cup \partial\Omega_T = \partial\Omega_m \cup \partial\Omega_\mu$, $\partial\Omega_u \cap \partial\Omega_\sigma = \partial\Omega_q \cap \partial\Omega_T = \partial\Omega_m \cap \partial\Omega_\mu = \emptyset$, and a bar over a quantity denotes its prescribed boundary value.

Then complementary generalized variational principles can be established. A potential energy type functional is constructed as:

$$\begin{aligned} \Pi(\mathbf{u}, \boldsymbol{\varepsilon}^r, \boldsymbol{\varepsilon}^i, \boldsymbol{\sigma}, \eta^r, T, c_\alpha, \mu_\alpha, \overset{q}{q}, \overset{T}{q}, \overset{m}{\alpha}, \overset{\mu}{\alpha}, \ell^{(\gamma)}, A^{(\gamma)}) \\ = E + \Phi - W + J_1 + J_2 + J_3 + J_4 + J_5 + J_6 \end{aligned} \quad (7)$$

where

$$\begin{aligned} E &= E(\boldsymbol{\varepsilon}^r, \eta^r, c_\alpha, \ell^{(\gamma)}) = \int_\Omega e^r(\boldsymbol{\varepsilon}^r, \eta^r, c_\alpha, \ell^{(\gamma)}) dV \\ \Phi &= \int_t \int_\Omega \left[\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^i + \overset{q}{q} \cdot \overset{T}{q} + \overset{m}{\alpha} \cdot \overset{\mu}{\alpha} + A^{(\gamma)} \dot{\ell}^{(\gamma)} - \phi^*(\boldsymbol{\sigma}, \overset{T}{q}, \overset{\mu}{\alpha}, A^{(\gamma)}) \right] dV dt \\ W &= \int_\Omega \mathbf{f} \cdot \mathbf{u} dV + \int_{\partial\Omega_\sigma} \bar{\mathbf{T}} \cdot \mathbf{u} dS - \int_t \int_{\partial\Omega_T} \bar{T} \overset{q}{q} \cdot \mathbf{n} dS dt - \int_t \int_{\partial\Omega_{\mu_\alpha}} \bar{\mu}_\alpha \overset{m}{\alpha} \cdot \mathbf{n} dS dt \\ J_1 &= \int_\Omega \left[\frac{1}{2}(\nabla \mathbf{u} + \mathbf{u} \nabla) - (\boldsymbol{\varepsilon}^r + \boldsymbol{\varepsilon}^i) \right] : \boldsymbol{\sigma} dV \quad J_2 = - \int_t \int_\Omega (\dot{\eta}^r + \nabla \cdot \overset{T}{q}) T dV dt \quad J_3 = - \int_t \int_\Omega (\dot{c}_\alpha + \nabla \cdot \overset{m}{\alpha}) \mu_\alpha dV dt \\ J_4 &= \int_{\partial\Omega_u} (\bar{\mathbf{u}} - \mathbf{u}) \cdot \boldsymbol{\sigma} \cdot \mathbf{n} dS \quad J_5 = \int_t \int_{\partial\Omega_q} T (\overset{q}{q} \cdot \mathbf{n} - \bar{J}_q) dS dt \quad J_6 = \int_t \int_{\partial\Omega_\alpha^m} \mu_\alpha (\overset{m}{\alpha} \cdot \mathbf{n} - \bar{J}_\alpha^m) dS dt \end{aligned}$$

Correspondingly, a complementary energy type functional is constructed as:

$$\begin{aligned} \Pi^*(\mathbf{u}, \boldsymbol{\varepsilon}^r, \boldsymbol{\varepsilon}^i, \boldsymbol{\sigma}, \eta^r, T, c_\alpha, \mu_\alpha, \overset{q}{q}, \overset{T}{q}, \overset{m}{\alpha}, \overset{\mu}{\alpha}, \ell^{(\gamma)}, A^{(\gamma)}) \\ = E^* + \Phi^* - W^* + J_1^* + J_2^* + J_3^* + J_4^* + J_5^* + J_6^* \end{aligned} \quad (8)$$

where

$$E^* = E^*(\boldsymbol{\sigma}, T, \mu_\alpha, A^{(\gamma)}) = \int_\Omega \left[\boldsymbol{\sigma} : \boldsymbol{\varepsilon}^r + T \eta^r + \mu_\alpha c_\alpha - A^{(\gamma)} \ell^{(\gamma)} - e^r(\boldsymbol{\varepsilon}^r, \eta^r, c_\alpha, \ell^{(\gamma)}) \right] dV$$

$$\Phi^* = \int_t \int_{\Omega} \left[\phi^* \left(\boldsymbol{\sigma}, \begin{matrix} T \\ q \end{matrix}, \begin{matrix} \mu \\ \alpha \end{matrix}, A^{(\gamma)} \right) \right] dV dt$$

$$W^* = \int_{\partial\Omega_s} \bar{\mathbf{u}} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} dS - \int_t \int_{\partial\Omega_q} T \bar{J}_q dS dt - \int_t \int_{\partial\Omega_m} \mu_\alpha \bar{J}_\alpha^m dS dt$$

$$J_1^* = \int_{\Omega} (\nabla \cdot \boldsymbol{\sigma} + \mathbf{f}) \cdot \mathbf{u} dV \quad J_2^* = - \int_t \int_{\Omega} \left(\begin{matrix} T \\ q \end{matrix} + \nabla T \right) \cdot \begin{matrix} q \\ \end{matrix} dV dt \quad J_3^* = - \int_t \int_{\Omega} \left(\begin{matrix} \mu \\ \alpha \end{matrix} + \nabla \mu_\alpha \right) \cdot \begin{matrix} m \\ \alpha \end{matrix} dV dt$$

$$J_4^* = \int_{\partial\Omega_\sigma} (\bar{\mathbf{T}} - \boldsymbol{\sigma} \cdot \mathbf{n}) \cdot \mathbf{u} dS \quad J_5^* = \int_t \int_{\partial\Omega_T} (T - \bar{T}) \cdot \begin{matrix} q \\ \end{matrix} \mathbf{n} dS dt \quad J_6^* = \int_t \int_{\partial\Omega_{\mu_\alpha}} (\mu_\alpha - \bar{\mu}_\alpha) \cdot \begin{matrix} m \\ \alpha \end{matrix} \mathbf{n} dS dt$$

It is obviously that $\Pi + \Pi^* = 0$ holds true so that the first variations of Π and Π^* satisfy $\delta\Pi = -\delta\Pi^*$. Considering the arbitrariness of $\delta\mathbf{u}, \delta\boldsymbol{\varepsilon}^r, \delta\boldsymbol{\varepsilon}^i, \delta\boldsymbol{\sigma}, \delta\boldsymbol{\eta}^r, \delta T, \delta \begin{matrix} T \\ q \end{matrix}, \delta \begin{matrix} \mu \\ \alpha \end{matrix}, \delta c_\alpha, \delta\mu_\alpha, \delta \begin{matrix} \mu \\ \alpha \end{matrix}, \delta \begin{matrix} m \\ \alpha \end{matrix}, \delta\ell^{(\gamma)}, \delta A^{(\gamma)}$, the sufficient and necessary conditions of following theorem is easy to prove.

Theorem: the first variation of Π or Π^* vanishes, if and only if $\mathbf{u}, \boldsymbol{\varepsilon}^r, \boldsymbol{\varepsilon}^i, \boldsymbol{\sigma}, \boldsymbol{\eta}^r, T, c_\alpha, \mu_\alpha, \begin{matrix} T \\ q \end{matrix}, \begin{matrix} \mu \\ \alpha \end{matrix}, \begin{matrix} m \\ \alpha \end{matrix}, \ell^{(\gamma)}, A^{(\gamma)}$ are the exact solution of above mentioned boundary value problem (1)~(6).

3 GIBBS T PE VARIATIONAL PRINCIPLE

With proper reduction, the proposed generalized variational principles become corresponding ones Kuang^[27-29] and Shen et. al^[23, 30-31] adopted. Those reduced form agree well with those theories reported in literature.^[27-35]

For one example, let first constitutive relations, second constitutive relations, gradient relations and Dirichlet boundary conditions be prescribed, that is taking (1)~(3) and (5) as preconditions. Thus, the thermo-chemo Gibbs type functional should be:

$$\Pi_g \left(\boldsymbol{\varepsilon}^r, \boldsymbol{\varepsilon}^i, T, \mu_\alpha, A^{(\gamma)} \right) = G^r + \Phi_g - W_g \quad (9)$$

where corresponding energy expressions for Gibbs type:

$$G^r = G^r \left(\boldsymbol{\varepsilon}^r, T, \mu_\alpha, A^{(\gamma)} \right) = \int_{\Omega} g^r \left(\boldsymbol{\varepsilon}^r, T, \mu_\alpha, A^{(\gamma)} \right) dV = \int_{\Omega} \left[e^r \left(\boldsymbol{\varepsilon}^r, \boldsymbol{\eta}^r, c_\alpha, \ell^{(\gamma)} \right) - T \boldsymbol{\eta}^r - \mu_\alpha c_\alpha + A^{(\gamma)} \ell^{(\gamma)} \right] dV$$

$$\Phi_g = \Phi_g \left(\boldsymbol{\varepsilon}^i, \begin{matrix} T \\ q \end{matrix}, \begin{matrix} \mu \\ \alpha \end{matrix}, A^{(\gamma)}, t \right) = \int_t \int_{\Omega} \left[\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^i - \phi^* \left(\boldsymbol{\sigma}, \begin{matrix} T \\ q \end{matrix}, \begin{matrix} \mu \\ \alpha \end{matrix}, A^{(\gamma)} \right) \right] dV dt$$

$$W_g = W_F - W_Q^* - W_C^* = \int_{\Omega} \mathbf{f} \cdot \mathbf{u} dV + \int_{\partial\Omega_\sigma} \bar{\mathbf{T}} \cdot \mathbf{u} dS + \int_t \int_{\partial\Omega_q} T \bar{J}_q dS dt + \int_t \int_{\partial\Omega_m} \mu_\alpha \bar{J}_\alpha^m dS dt$$

g^r represents the Gibbs free energy density here.

Then

$$\begin{aligned} \delta\Pi_g = & \int_{\partial\Omega_\sigma} (\boldsymbol{\sigma} \cdot \mathbf{n} - \bar{\mathbf{T}}) \cdot \delta\mathbf{u} dS - \int_{\Omega} (\nabla \cdot \boldsymbol{\sigma} + \mathbf{f}) \cdot \delta\mathbf{u} dV + \int_t \int_{\partial\Omega_q} \left(\begin{matrix} q \\ \end{matrix} \cdot \mathbf{n} - \bar{J}_q \right) \delta T dS dt \\ & + \int_t \int_{\partial\Omega_m} \left(\begin{matrix} m \\ \alpha \end{matrix} \cdot \mathbf{n} - \bar{J}_\alpha^m \right) \delta\mu_\alpha dS dt - \int_t \int_{\Omega} \left(\dot{c}_\alpha + \nabla \cdot \begin{matrix} m \\ \alpha \end{matrix} \right) \delta\mu_\alpha dV dt - \int_t \int_{\Omega} \left(\dot{\boldsymbol{\eta}}^r + \nabla \cdot \begin{matrix} q \\ \end{matrix} \right) \delta T dV dt \end{aligned} \quad (10)$$

Considering thermodynamic reversible strain $\boldsymbol{\varepsilon}^r = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^i$, current concentration $\tilde{c}_\alpha = c_\alpha + r_\alpha = c_\alpha + v_\alpha^{(\gamma)} \ell^{(\gamma)}$, chemical affinity $A^{(\gamma)} = -\mu_\alpha v_\alpha^{(\gamma)}$ and dissipative power $\dot{\psi}(\eta^i) = T\dot{\eta}^i$ with $\dot{\eta} = \dot{\eta}^r + \dot{\eta}^i$, one has

$$\begin{aligned} g^r(\boldsymbol{\varepsilon}^r, T, \mu_\alpha, A^{(\gamma)}) &= e^r(\boldsymbol{\varepsilon}^r, \eta^r, c_\alpha, \ell^{(\gamma)}) + \psi - T\eta^r - \mu_\alpha c_\alpha + A^{(\gamma)} \ell^{(\gamma)} - T\eta^i + T\hat{\eta}^i \\ &= e(\boldsymbol{\varepsilon}^r, \eta, \tilde{c}_\alpha) - T\eta - \mu_\alpha \tilde{c}_\alpha + T\hat{\eta}^i = g_c(\boldsymbol{\varepsilon}^r, T, \mu_\alpha) + T\hat{\eta}^i \\ \psi_g &= \int_t \left[\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^i - \phi^* \left(\boldsymbol{\sigma}, \frac{T}{q}, \mu_\alpha, A^{(\gamma)} \right) \right] dt = \int_t \dot{d}_{gc} dt = d_{gc} \end{aligned} \quad (11)$$

in which a superposed hat (^) denotes a variable to be held fixed during variation, $g_c(\boldsymbol{\varepsilon}^r, T, \mu_\alpha)$ and d_{gc} are respectively the Gibbs free energy density and corresponding dissipative energy density that Kuang^[27-29] and Shen et. al^[23, 30-31] adopted. The reduced form deduced here equals to the Gibbs type quasi variational principle for multi-field problem that Kuang and Shen proposed.

It's important to emphasize that, Yu and Shen^[30] introducing quasi variational term $\delta\hat{Q}^* = -\int_\Omega \hat{\eta}^i \delta T dV$ of (11) into the heat source term δB_Q^* , by the interpretation of “the irreversible part of the complement of heat corresponding to the inner complement dissipative energy”^[23]. That term ingeniously avoid energy imbalance during deducing principles from free energy density g_c and dissipative energy density d_{gc} separately. However, derivation in this section shows that the division of total internal energy simplifies the formulas and derivation of variational principles significantly. And a variational principle with an explicit functional has great advantage than those quasi variational principles in future application.

4 NUMERICAL EXAMPLE

To illustrate the main progress in present approach, we consider a chemical active thin plate bonded to a rigid substrate, immersed in a liquid as Fig.1. This plate deforms gradually due to chemical reaction and mass diffusion on isothermal assumption. Assuming we have linear constitutive laws, such a chemo-mechanical coupling problems can be described in a weak-form of equivalent integral equation based on the theoretical model mentioned above. Solved by PDE toolbox of COMSOL Multi-physics[®], the displacement distributions in the normal direction during different reaction-diffusion process are shown in Fig.2.

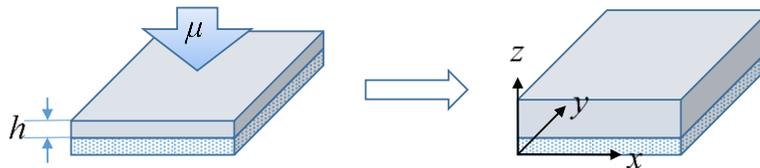
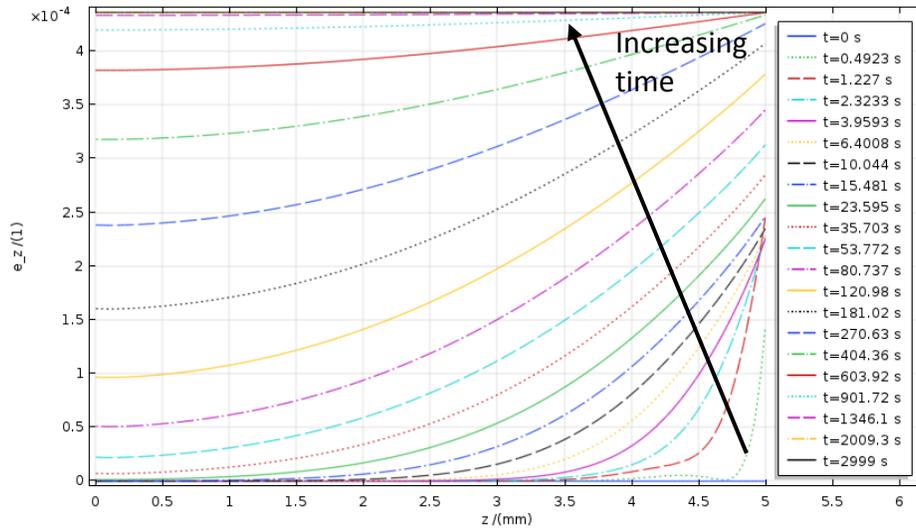
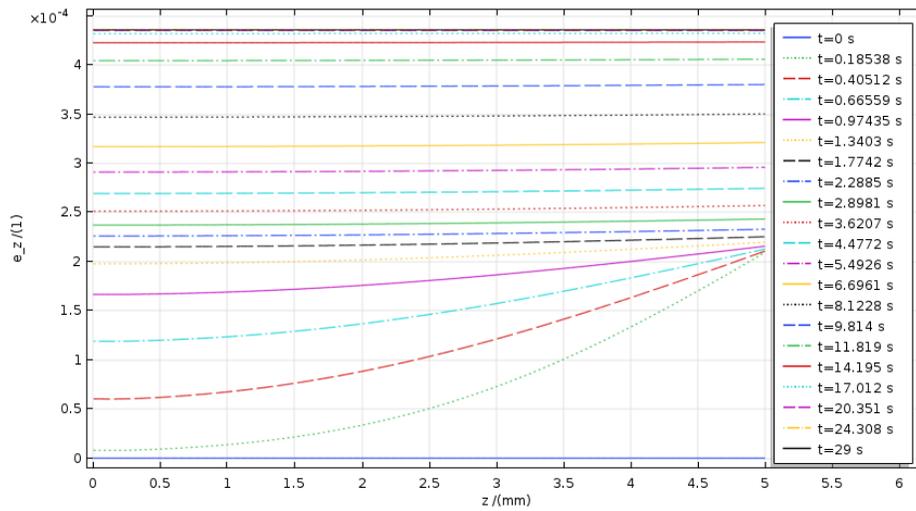


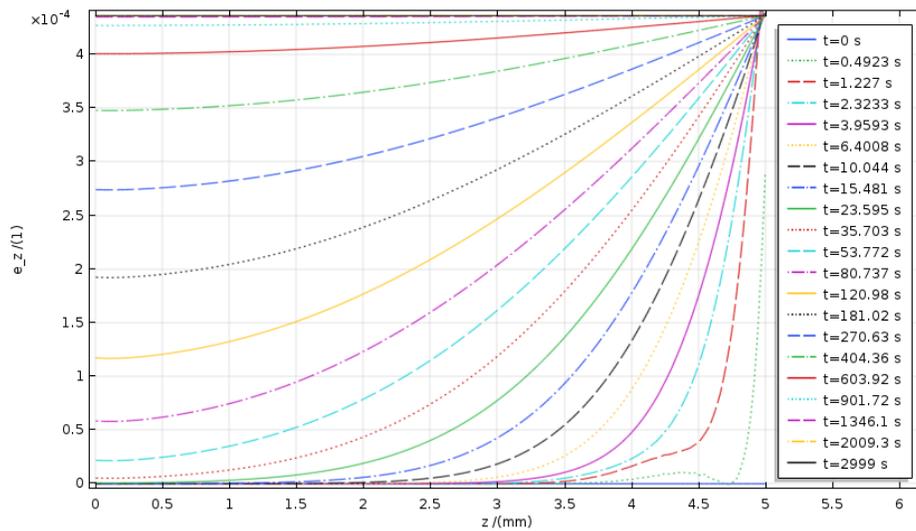
Fig.1 Schematic diagram



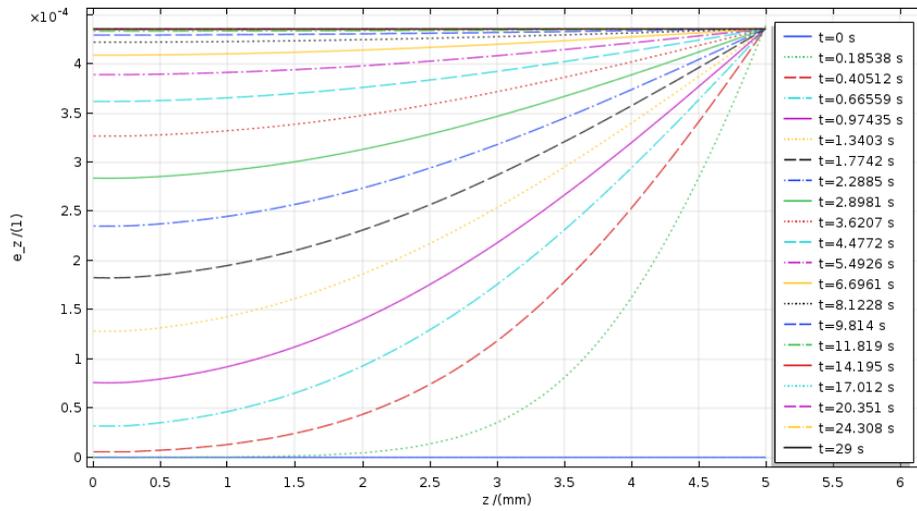
(a) $D=4e-7$ [mol²/(m³J*s)], $knct=2e-3$ [1/s]



(b) $D=4e-5$ [mol²/(m³J*s)], $knct=2e-3$ [1/s]



(c) $D=4e-7$ [mol²/(m³J*s)], $knct=2e1$ [1/s]



$$(d) D=4e-5[\text{mol}^2/(\text{m}^*\text{J}\cdot\text{s})], knct=2e1[1/\text{s}]$$

Fig.2 Displacement u_z distribution in z direction for different reaction-diffusion process

Results in Fig.2 indicate the different evolving process under different diffusion rate (measured by diffusion coefficient D) and different reaction rate (measured by reaction rate constant $knct$). Fig.2(b) reveals a typical reaction control process while Fig.2(c) a diffusion control process. Fig.2(a) and Fig.2(d) present the competition of contributions from diffusion and chemical reaction in different time scale. Such results agree well with those analytical conclusions of Zhang and Zhong^[24].

CONCLUSIONS

- Two complementary generalized variational principles for fully coupled thermo-chemo-mechanical problems are established. Discussion on simplification to theories in literature indicates the conciseness of proposed theory.
- Simulations show that weak-form integral equations based on the theoretical model mentioned above is suitable for simulating such multi-physics problems. This approach reveals the difference under different process.

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Large-scale and Parallel Pre-processing Researches and SuperMesh Development

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ABSTRACT

One of the key technologies to improving the availability of high performance numerical simulation is the large-scale and parallel pre-process technology, which serves to generate large-scale, high precision and high resolution grids quickly and with high quality. Facing the challenge of whole system and three-dimensional simulation running on peta-flop supercomputer, and in order to meet the needs of 'cloak meshing', the pre-processing engine SuperMesh is developed. We presents an accurate and highly automatic geometry processing and mesh generation pipeline of SuperMesh and its flexible extensible architecture here, which could generates large-scale structured and unstructured mesh for complicated CAD Model, and could be butted seamlessly with the parallel programming framework JASMIN, JAUMIN and JCOGIN. Since 2013, SuperMesh has been used in customizing specific packages for several high performance numerical simulation software based on those programming framework. Currently, in order to face the challenge of 100 peta-flop computing, researches have been carried out in automatic model cleaning based on mixed representation and multilevel parallel mesh generation. Firstly, mixed representation of Brep model and discrete model is used to change Brep model synchronously when processing discrete model for coordinated mesh generation. Then, Brep model partition and mesh size prediction method are applied in first level parallel mesh generation. Finally, a background mesh partition method is used and the subsequent steps of surface meshing, volume meshing and mesh improvement in sub-region are executed in a complete parallel manner, all these related novel algorithms are going to be incorporated in SuperMesh. References [1] Jianjun Chen, Zhiwei Liu, Yao Zheng, Peng Zheng, Jianjing Zheng, Zhoufang Xiao, Chuang Yu. Automatic sizing ?functions for 3D unstructured mesh generation. Procedia Engineering, (In: Proc. of the 26th International Meshing Roundtable, Barcelona, Spain, Sep 18-21 2017) 2017; 203: 245-257. [2] Zeyao Mo, Aiqing Zhang, Xiaolin Cao, Qingkai Liu, Xiaowen Xu, Hengbin An, Wenbing Pei, Shaoping Zhu. JASMIN: a parallel software infrastructure for scientific computing[J], Front. Comput. Sci. China, 4(4): 480-488, 2010. [3] Peng Zheng, Wei Fang, Quan Xu, Juelling Leng, Min Xiong, Changhua Yu. Parallel AFT Tetrahedral Mesh Generation for JAUMIN[J/OL]. Journal of Frontiers of Computer Science and Technolgy, [2017-12-21].<http://kns.cnki.net/kcms/detail/11.5602.TP.20170103.1036.006.html>.

The Numerical Study of Phase Transition of Temperature Sensitive Hydrogel under Mechanical Constraint

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ABSTRACT

The numerical study of phase transition of temperature sensitive hydrogel under mechanical constraint Shoujing Zheng, Zishun Liu* International Center for Applied Mechanics, State Key Laboratory for Strength and Vibration of Mechanical Structures, Xi'an Jiaotong University, Xi'an, 710049, People's Republic of China *Corresponding Author: zishunliu@mail.xjtu.edu.cn Abstract Temperature sensitive hydrogel is blessed with outstanding properties which may be utilized for innovative appliance. However, this is not achievable if the phase transition property of it is not well understood. Under certain mechanical constraint or temperature stimuli, the hydrogel shows the phase transition, a very special phenomenon that shows huge volume change. Based on the theory that can predict this volumetric deformation, we developed a numerical method to study the phase transition under mechanical constraints. In the simulation, the subroutine of ABAQUS is used to calculate the stress of the hydrogel under the uniaxial load. The subroutine is in the UHYPER form, which is developed by our group previously (Ding et al., 2013). Using the code, we found that the mechanical behavior is intrinsically different before and after the phase transition. We also found that near the phase transition, multiple curves can be obtained in the stress-stretch figure. In other words, near the phase transition region, one stress can correspond to at least two stretches, one representing the swollen state, one representing the shrunk state. The calculation above can prove the existence of phase transition numerically. Furthermore, using Dynamic Mechanical Analysis, we have conducted experiments to quantitatively investigate this peculiar behavior. Based on the experimental data, a new decision rule is formulated to determine the critical stress. Finally, with a proper fitting parameter and a transformation from referential state to free swelling state, we can compare the numerical prediction of the stress-stretch curve with results from experiments (Zheng and Liu, 2017). References Ding, Z., Liu, Z., Hu, J., Swaddiwudhipong, S., Yang, Z., 2013. Inhomogeneous large deformation study of temperature-sensitive hydrogel. International Journal of Solids and Structures 50, 2610-2619. Zheng, S., Liu, Z., 2017. Phase transition of temperature sensitive hydrogel under mechanical constraint. Journal of Applied Mechanics.

Extended Multiscale Finite Element Methods for the Localization and Crack Propagation Analyses of Heterogeneous Materials

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ABSTRACT

Based on the embedded strong discontinuity model, we have developed recently the extended multiscale finite element methods for the strain localization and crack propagation analyses of homogeneous and heterogeneous materials. In these methods, the kinematic descriptions of the localization and crack are considered based on a set of fine-scale meshes with the strong discontinuity model. Then an enhanced coarse element strategy, in which additional coarse nodes can be adaptively added according to the propagation of shear band or discontinuity line, is used to construct the multiscale numerical base functions that can well capture the localization or discontinuous characteristics and transform the information between the fine scale and coarse scale. The mechanical problems are then solved in a coarse-scale mesh by upscaling from the fine-scale meshes based on the developed enhanced coarse element strategy. The displacement decomposition technique is adopted to modify the downscale computations by adding the perturbation solutions and thus the microscopic displacement can also be accurately obtained. Various representative numerical examples were carried out to demonstrate the effectiveness and high efficiency of the proposed methods. References [1] Lu, M.K.; Zhang, H.W.; Zheng, Y.G.*; Zhang, L. A Multiscale Finite Element Method for the Localization Analysis of Homogeneous and Heterogeneous Saturated Porous Media with Embedded Strong Discontinuity Model. *Int. J. Numer. Methods Eng.*, 2017, 112, 1439. [2] Lu, M.K.; Zhang, H.W.; Zheng, Y.G.*; Zhang, L. A Multiscale Finite Element Method with Embedded Strong Discontinuity Model for the Simulation of Cohesive Cracks in Solids. *Comput. Methods Appl. Mech. Eng.*, 2016, 311, 576. [3] Zhang, H.W.*; Lu, M.K.; Zheng, Y.G.; Zhang, S. General Coupling Extended Multiscale FEM for Elasto-Plastic Consolidation Analysis of Heterogeneous Saturated Porous Media. *Int. J. Numer. Anal. Methods Geomech.*, 2015, 39, 63.

Investigation of Thermal Alleviation on Cold Dwell Fatigue

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ABSTRACT

Dwell sensitivity is well known in titanium alloys, and is found to cause high peak stresses that can lead to failure. The mechanism of dwell debilit is thought to be related to very particular crystallographic orientation combinations. A polycrystalline aggregate containing a combination of a primary hard grain with c-axis nearly parallel to the loading direction and adjacent soft grains with c-axis nearly normal to the loading direction, commonly known as a rogue grain combination, was studied under a dwell fatigue condition using crystal plasticity model with dual phase morphology explicitly represented. Load shedding was found to occur within the rogue grain combination, in which stress is redistributed from the soft grain to the hard grain during a hold at peak applied stress. Load shedding was also found to be strongly affected by temperature: the amount of stress redistribution is significantly reduced when temperature increased from 20°C to 300°C. The temperature sensitivity of load shedding is a result of the diminishment in strain rate sensitivity at high temperatures. Engine rig spin tests under isothermal conditions and realistic in-service engine loading histories (non-isothermal) was modelled and compared using dual phase polycrystal model. The evolution of effective plastic strain and dislocation density around the hard-soft grain boundary was captured and quantified. The peak stress developed during the loading under in-service conditions was found to be lower than the critical value to initiate facet crack due to the inhibition of load shedding at high temperature.

Study on Sharp V-notch Problem Using Symplectic Analytical Singular Element

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ABSTRACT

V-notch problem with dynamic loading condition is considered in this paper. In the time domain, the precise time domain expanding algorithm is employed, in which a self-adaptive technique is carried out to improve computing accuracy. By expanding variables in each time interval, the recursive finite element formulas is derived. In the space domain, a Symplectic Analytical Singular Element (SASE) is constructed within the framework of finite element method (FEM). The vicinity of the crack tip is represented by using the SASE, and the other area is meshed by using conventional elements. Due to the advantage of the SASE, the dynamic stress intensity factors (DSIFs) can be obtained directly via the relationship between the the eigen expanding coefficients and the DSIFs, without any post-processing. Numerical examples are conducted to investigate the accuracy and the stability. Results show that the proposed SASE for dynamic V-notch problem is effective and efficient.

In-vivo Effects of Different Orthodontic Loading on Root Resorption and Correlation to Mechanobiological Stimulus in Periodontal Ligament

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ABSTRACT

Orthodontic root resorption (ORR) is a common side effect of orthodontic therapy. In orthodontic practice, the treatment-related risk factors are of particular interest to clinicians, and orthodontic load magnitude is believed to be one of the primary controlling factors. High pressure in the periodontal ligament (PDL) generated by orthodontic forces will trigger recruitment of odontoclasts, leaving resorption craters on root surfaces. However, due to intricate anatomical and physiological environment for ORR, odontoclast's in-vivo responses to mechanobiological loading have yet to be studied. The patterns of resorption craters are the traces of odontoclast activity. Therefore, this study aimed to investigate the mechanobiological relationship influencing the extent and distribution of orthodontic root resorption, considering the resorptive patterns as evidences of in-vivo cellular responses to two different levels of orthodontic loadings. First, the resorption craters were quantitatively assessed in a 3D manner using microCT. The spatial information and individual crater characteristics were analysed to provide insights into in-vivo odontoclast activities and their patterns, with reference to known regulations of osteoclast behaviour. Furthermore, 3D subject-specific nonlinear finite element (FE) models were created based on the microCT images to evaluate the corresponding mechanobiological stimuli induced by different orthodontic loadings. With combination of experimental and numerical characterisation, the correlation between ORR and orthodontic loading can be analysed. Results indicated that the heavy force (225 g) led to a larger total resorption volume than the light force (25 g), mainly by presenting larger individual crater volumes ($p < 0.001$) than increasing crater numbers, suggesting that increased mechano-stimulus predominantly boosted cellular resorption activity rather than recruiting more odontoclasts. Furthermore, buccal-cervical and lingual-apical regions in both loading groups were found to have significantly larger resorption volumes than other regions ($p < 0.005$). These clinical observations are complimented by the finite element analysis (FEA) results, which indicated that when the volume average compressive hydrostatic pressure exceeded the capillary blood pressure (4.7kPa), root resorption was more likely to be induced. This work provides new insights into the odontoclastic activities in-vivo and helps in predicting therapeutical outcomes, for potential improvement in the generally sophisticated surgical procedure.

Dual-basis Dimensional Reduction for Non-dissipative Explicit Dynamic Discrete Element Simulations with High-frequency Noises

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ABSTRACT

We present, for the first time, a dimensional reduction model based on proper orthogonal decomposition (POD) for non-dissipative explicit dynamic discrete element method (DEM) simulations. Two individual POD bases are obtained by the method of snapshots for the displacement and rotation degrees of freedom of the discrete element particles, respectively. The POD basis for rotation is extracted from the vector space of angular velocity. Since the rotation vectors are pseudovectors which adopt a different algebra, explicit Lie-group time integrator is introduced for the integration of particle rotations, while the time integrator for the displacement field is in the Euclidean space. As such, the two set of snapshots are taken from the simulations with numerically dissipative schemes. Then the derived reduced dimension bases are employed in energy-momentum conserving DEM simulations. This approach brings four important benefits. First, one may filter out the high-frequency noises and obtain accurate results without introducing artificial damping that sometimes leads to inconsistent results and reduced wave propagation speed. Second, the number of snapshots used for displacement and rotation can be different, depending on the nature of the problems. Third, since this method requires no injection of artificial or numerical damping, there is no need to tune damping parameters. Finally, the suppression of high-frequency responses allows larger time step for faster explicit integration. The proposed POD-DEM scheme is important for analyzing wave propagation, mixing, rate-dependent simulations for particular materials in which how the external work applied on the system converts into internal energy and dissipation are critical to the outcomes.

Simulation of Crack Growth by Method of Updating Sub-partition and Substructure

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ABSTRACT

A method of updating sub-partition and substructure in finite element frame is proposed to simulate the crack propagation in planar and plate structures. Using this method crack configuration is modeled independently to global element mesh. The element cut apart by crack is sub-partitioned into ordinary sub-elements while an element cut into by crack tip is sub-partitioned into several singular sub-elements. Whole sub-partitioned elements which overlap a crack constitute a substructure. The sub-partition and substructure is updated (or to be generated) corresponding to the propagation of existing crack grows (or nucleation of a new crack). In this way global re-meshing is avoided for FE simulating crack extension along arbitrary path or crack initiating anywhere. The additional nodal freedom degrees introduced by element sub-partition in the substructure are condensed to boundary nodes of the substructure which are just the original mesh nodes. Thus, freedom degrees of global structure analysis are invariable. The proposed method is within ordinary FEM frame, so all the existing constitutions of material and models of element can be employed directly. It avoids the difficulty of formulating asymptotic function at crack tip for non-linear problems which conventional XFEM faces with. 5-node singular planar and shell elements are constructed to represent the singularities at crack tips for planar and plate bending problems, respectively. These elements connect with the ordinary four-node linear planar or plate elements directly. The proposed method and singular elements are used in fracture analysis for both planar and plate bending structures. Good accuracy of the crack tip fields prediction and good adaptability of moving crack simulation are demonstrated through examples.

Progressive Failure Modelling for Heterogeneous Media with Strain Strength Distribution and Microplane Model

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ABSTRACT

A progressive damage model based on strain strength distribution criterion and microplane model is proposed. In the strain strength distribution criterion (Li & Zhou, 2013), the strain strength of the heterogeneous material is assumed to be distributive in space in mesoscopic view. Thus in the failure process, fracture plane in any direction of the representative volume element (RVE) for the material is considered to be composed of elastic area and fracture area. The interactions on the elastic area remains elasticity, while on the fracture plane it turns into contact and complies with the Coulomb's friction law. The ratio of the fracture area to the total area of the fracture plane is defined as the fracture degree, which can be explicitly and quantitatively expressed with a certain distribution function. In the 3D microplane model (Brocca, Brinson & Bažant, 2002), the stress-strain relations are defined independently on planes of all possible orientations in the microstructure. Different constitutive laws for the microplane are defined and proposed. However, the reasonable model with specific physical meaning and being capable of describing the heterogeneous properties are still need to be developed. The progressive damage model proposed in this paper combines the advantages of the above two models. The framework of the model is established with the principle of virtual work that is similar to the microplane model. A spherical RVE is defined and the stress-strain relationship in any direction of the spherical surface is given by the strain strength distribution model. There are no artificial parameters introduced in this model except the distribution function of the strength within the material. Theoretical and numerical results show that, if the material is not damaged, the model will degenerate into the 3D generalized Hooke's law, while in the failure process, the nonlinear and strain softening can be naturally obtained. Li S, Dong Z. Progressive failure constitutive model of fracture plane in geomaterial based on strain strength distribution [J]. International Journal of Solids & Structures, 2013, 50(3-4):570-577. Brocca M, Brinson L C, Bažant Z P. Three-dimensional constitutive model for shape memory alloys based on microplane model [J]. Journal of the Mechanics & Physics of Solids, 2002, 50(5):1051-1077.

A Non-ordinary State-based Godunov-Peridynamics Formulation for Shocks in Solids

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ABSTRACT

The theory and meshfree implementation of Peridynamics has been proposed to model problems involving strong transient discontinuities such as impact-induced fragmentation. For effective application of numerical methods to these events, essential shock physics and Gibbs instability should also be addressed. So far, the artificial viscosity technique has been employed [1-3] in Peridynamics to treat shocks. This technique is simple to implement, but involves tunable parameters which is undesirable, and can lead to results which are not objective. On the other hand, the Godunov scheme has been shown to be an effective approach for shock modeling which does not involve any tunable parameters and directly embeds shock physics into the formulation with the Gibbs instability addressed in an effective way. However, this scheme was originally developed based on mesh-based frameworks, and to incorporate it into meshfree methods such as Peridynamics is not straightforward. This work introduces a physics-based shock modeling formulation for non-ordinary state-based Peridynamics, in which Godunov scheme is introduced by embedding Riemann solution into the force state. Several benchmark problems are solved with high accuracy to demonstrate the effectiveness of the proposed formulation. [1] Ren, B., Fan, H., Bergel, G.L., Regueiro, R.A., Lai, X. and Li, S., 2015. A peridynamics–SPH coupling approach to simulate soil fragmentation induced by shock waves. *Computational Mechanics*, 55(2), pp.287-302. [2] Lai, X., Liu, L., Li, S., Zeleke, M., Liu, Q. and Wang, Z., 2018. A non-ordinary state-based peridynamics modeling of fractures in quasi-brittle materials. *International Journal of Impact Engineering*, 111, pp.130-146. [3] Silling, S.A., Parks, M.L., Kamm, J.R., Weckner, O. and Rassaian, M., 2017. Modeling shockwaves and impact phenomena with Eulerian peridynamics. *International Journal of Impact Engineering*, 107, pp.47-57.

Shape Identification for Inverse Geometry Heat Conduction Problems by FEM without Iteration

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ABSTRACT

The boundary geometry shape is identified by the finite element method (FEM) without iteration and mesh reconstruction for two-dimensional (2-D) and three-dimensional (3-D) inverse heat conduction problems. Firstly, the direct heat conduction problem with the exact domain is solved by the FEM and the temperatures of measurement points are obtained. Then, by introducing a virtual boundary, a virtual domain is formed. By minimizing the difference between the temperatures of measurement points in the exact domain and those in the virtual domain, the temperatures of the points on the virtual boundary are calculated based on the least square error method and the Tikhonov regularization. Finally, the objective geometry shape can be estimated by the method of searching the isothermal curve or isothermal surface for 2-D or 3-D problems, respectively. In the process, no iterative calculation is needed. The proposed method has a tremendous advantage in reducing the computational time for the inverse geometry problems. Numerical examples are presented to test the validity of the proposed approach. Meanwhile, the influences of measurement noise, virtual boundary, measurement point number and measurement point position on the boundary geometry prediction are also investigated in the examples. The solutions show that the method is accurate and efficient to identify the unknown boundary geometry configurations for 2-D and 3-D heat conduction problems.

Design for Additive Manufacturing

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ABSTRACT

In recent years additive manufacturing, in popular term 3D-Printing, has become a broad technology movement. By large its fame is driven by rapidly growing consumer adoption. However, rapid growth has been seen in biomedical applications, and initial successes have also been showcased for aerospace and other fields. 3D-Printing brings almost unlimited freedom for design shape and form, hence offers the perfect combination with topology optimization for creation of most efficient structures. Many successful designs created with topology optimization have been presented in real product environment by leading global companies. In recent years the authors have developed several advanced features in OptiStruct to address unique needs from additive manufacturing. These include: (1) design of blended solid/lattice structures; (2) topology optimization considering support elimination or penalization. This paper offers a general treatment around design for additive manufacturing, including software tools for final geometry creation and printing processing. We will also discuss further development of optimization capabilities including dual utilization of lattice serving both structural and printing support purposes.

Topology Optimization of Coupled Thermofluidic-mechanical Problems for Channel-cooling Structures

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ABSTRACT

This work introduces an efficient topology optimization approach for coupled thermofluidic-mechanical problems to design structures containing straight cooling channels. Instead of using a full-blown but computationally expensive thermofluidic solver, a simplified thermofluidic model together with a multiphase parameterization based on the Solid Isotropic Material with Penalization (SIMP) model are developed to design the cross section of the device that consists of solid, fluid and void. A design dependent convection boundary scheme is proposed to allow continuous interpolation of heat sinks among multi-phases for topological design as well as a pertinent thermofluidic simulation. Numerical examples which take engineering requirements on lightweight, uniform structural deformation and temperature distribution into account are given to demonstrate the applicability of the approach. Verifications of the optimized 3D structures by a full-blown thermofluidic simulation show that the proposed approach can yield lightweight channel-cooling structures with desirable heat-transfer and load-carrying performances subject to external heat flux and static load.

Damage Resistance Properties of Hybrid Fiber Reinforced Magnesium Alloy Laminates Subjected to Low Velocity Impact

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ABSTRACT

In order to investigate the low-velocity impact response of novel fiber reinforced magnesium alloy laminates, the numerical simulations of low velocity drop weight impact tests on AZ31B magnesium alloy laminates reinforced with glass fiber, carbon fiber and their hybrids under different impact energies were conducted. The simulation predictions are also compared with the existing experimental results [1]. The magnesium alloy, the interfacial delamination between two neighboring layers and the fiber/epoxy composites in the fiber/AZ31B Mg laminates were modeled through an anisotropic plastic constitutive model, an exponential cohesive zone model, and 3D Hashin failure criteria incorporated with the stiffness reduction of failed elements respectively. In addition, the numerical analyses of low-velocity impact for different fiber/Mg alloy laminates were carried out by using ABAQUS/Explicit with a user-defined subroutine (VUMAT) to predict the dynamic impact response and delamination as well as damage evolution rules under conditions of different impact energies. Meantime, the variations of impact force, deformation and energy absorption with time were also analyzed. The results show that the matrix cracking for different fiber/Mg alloy laminates firstly occurred in the backside at the lower impact energy (20J), while the matrix cracking and fiber breakage could also appear in the impact side as the impact energy increases from 20 J to 50 J. Compared with the single carbon fiber/Mg alloy laminate, the single glass fiber/Mg alloy laminate can absorb more energy under an impact load. Hybrid carbon fiber and glass fiber reinforced Mg alloy laminates can improve the impact-resistant properties when the glass-fibers plies are set at the appropriate layers. When the impact energy is in the range of 20-50 J and the glass-fibers plies are located on the second layer of 3/2 hybrid fiber/Mg alloy laminates, the hybrid carbon fiber and glass fiber reinforced Mg alloy based laminates have the best impact toughness and good impact damage resistance properties. The simulation and experimental results are in good agreement in terms of the damage morphology, the curves of force-time and force-deflection. The mechanical response and the damage trends of the fiber magnesium laminates under low velocity impact can be well predicted using the VUMAT subroutine. [1] T. Pärnänen, R. Alderliesten, C. Rans, T. Brander, O. Saarela. Applicability of AZ31B-H24 magnesium in Fibre Metal Laminates – An experimental impact research [J]. Composites Part A Applied Science & Manufacturing, 2012, 43(9):1578-1586.

Ultralight and Super-elastic Honeycomb Plate of Graphene Aerogel

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ABSTRACT

Graphene is a one-atom-thick layer of carbon atoms arranged in a hexagonal pattern, which makes it the strongest material in the world. Controlled preparation of graphene aerogel from graphene can be achieved by freeze-drying, self-assembly, template growth and 3D printing. In this paper, a continuous honeycomb plate out of graphene aerogel was presented and analyzed. In the honeycomb plate, the framework of the plate is used as the template for unidirectional growth of the graphene aerogel. Then, multiscale simulations were performed on the honeycomb plate by combining finite element method and coarse-grained molecular dynamics method. Firstly, a coarse-grained molecular dynamics model of the honeycomb plate of graphene aerogel was built. The cyclic compressive and bending tests of a unit cell of the honeycomb plate were simulated to study its mechanical properties and microstructural evolution. Then, the deformation response of plate was simulated using ABAQUS. The results showed that the plate is able to recover its initial shape even after large deformation. It is attributed to the three-dimensional honeycomb structure and the graphene aerogel microstructure.

Dual-anisotropic Solid Metamaterials for Elastic Wave Manipulation

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ABSTRACT

Dual-anisotropic solid materials refer to those with anisotropic stiffness and anisotropic inertial density simultaneously. They are found to be vital to the realization of elastic wave control according to the transformation elasticity theory. In this study, we propose a new type of structured metamaterials with the dual-anisotropic property. The proposed metamaterial is a periodic composite material, with the unit cell consisting of the stiff hexagonal lattice serving as the host, in which the soft two-bar inclusions are embedded. The anisotropic stiffness can be acquired by tailoring the geometry of the hexagonal lattice. The sharpened bar inclusion is designed by mimicking the slipping-boundary effect in fluid-solid interfaces in order to pursue the broadband anisotropic inertial density. We have developed an effective-medium model to retrieve the effective stiffness and density from the band-structure results. Effective-medium results verify the almost constant dual-anisotropic properties achieved in the broad frequency range. The cloaking structure is a device that can prevent elastic wave penetration into its interior. Based on the linear-transformation mapping, we construct a carpet cloaking device and derive the dual-anisotropic material parameters from the transformation method. Based on the proposed model, we design the metamaterial elements that fulfill the parameter requirement and assemble them into the cloaking structure. Numerical simulations show that the interior strain field amplitude can be greatly lowered in the broad frequency range due to the protection of the metamaterial cover. Our studies are expected to open a new route to the broadband elastic wave mitigation using dual-anisotropic solid metamaterials. Reference: Yong Cheng, Xiaoming Zhou, and Gengkai Hu, Broadband dual-anisotropic solid metamaterials, Scientific Reports, 7, 13197, 2017.

Examples of Uncertainties of Molecular Dynamics Simulations

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ABSTRACT

Properties of materials always exhibit variabilities due to the statistical nature of microstructural details. Understanding such variabilities is critical for engineering design. Unfortunately, material models usually create additional variabilities due to the statistical nature of numerical procedures. It is therefore challenging to model the microstructure-induced variabilities without first reducing the model-induced variabilities. Here we discuss the variabilities commonly created by molecular dynamics models using three examples: dislocation energy calculations, diffusion studies, and vapor deposition simulations. Counter-intuitively, we found that molecular statics simulations can create much larger variabilities than molecular dynamics simulations especially for large systems containing many metastable states. In some cases, the variabilities of time-averaged molecular dynamics simulations can be reduced to almost zero. In other cases where the variabilities are not zero, molecular dynamics simulations can still provide convincing insights that help improve materials in experiments. Acknowledgement: Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

Kinetic Analysis of Multi-DOF Motion Simulator

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ABSTRACT

This thesis studies on the multi-degree of freedom electro-hydraulic hybrid turntable, which composed by the six-DOF parallel turntable (Stewart turntable) and three-axis turntable. The upper body in the Stewart platform can realize six-DOF movement in the space through six hydraulic drive lever; outer ring, central ring and inner ring(working space) of three-axle table can infinitely rotate in any orientation space. The establishment of Hybrid Turntable, comprehensive two kinds of platforms, realizes the control in any positions and any directions, which not only compensates range limits of Stewart platform rotation, but also to make up the bound that three-axis turntable cannot move randomly, making the study more theoretical significance and the actual value. This paper analyzes the multi-degree of freedom electro-hydraulic hybrid turntable from kinematics and dynamics aspects, the kinematics and dynamics equations are obtained; using the software program of MATLAB to the motion model for motion simulation and dynamic simulation and draw simulation graphs, And then through analyzing and summarizing, draw conclusions. The simulation results coincide with the actual motion of simulator. The results obtained would be useful for the design and analysis of practical manufacture.

A Study of Stress Singularities Arising at the Interface in One-Dimensional Hexagonal Piezoelectric Quasicrystals

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ABSTRACT

Quasicrystals (QCs) are a special class of quasi-periodic alloys which possess a series of ideal properties such as high hardness, low adhesion, low coefficient of friction, low porosity, low electrical and thermal conductivity. Due to their piezoelectric effects, QCs can be used in manufacturing the sensor and actuator in the smart systems. The present study proposed a simple method for the determination of fracture parameters of the one-dimensional hexagonal piezoelectric QC with an interface V-notch. The present method is carried out in two steps. In the first step, the physical domain is meshed by the conventional element for QCs and is divided into a finite size singular region near the notch tip and a regular region far away from the notch tip. In the second step, exact solution of V-notched QCs which can be represents by a series of analytical symplectic eigenfuntions is derived by establishing a Hamiltonian system. By using the obtained solutions, the large number of nodal unknowns in the singular region are transformed into a small set of undetermined coefficients of a symplectic series. The nodal unknowns in the regular region remain as usual. Consequently, high-accuracy generalized intensity factors are obtained by the first several coefficients of the series. Explicit expressions in the singular fields are obtained simultaneously. Numerical results are compared with the existing solutions and found to be in good agreement. Some new results are given also. Compared with other numerical methods, the present has three advantages. First, based on the symplectic eigenfunction expansion of the near region, the number of unknown variables is reduced to a very low level. This results in reducing the computational time and the memory requirement for fracture analysis of cracked structures. Second, no special finite elements and post-processing are needed to determine the generalized intensity factors and the exact solutions in the near fields are obtained simultaneously. Third, as the analytical solution is embodied in the transformation, the accuracy of the predicted generalized intensity factors and their derivatives is high.

Control Acoustic Wave at the Deep Sub Wavelength Scale with Anisotropic Metasurface

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ABSTRACT

Manipulating acoustic wave at the deep sub wavelength scale is of great interests. In this talk we introduce the design of gradient-index metasurface that can manipulate airborne acoustic wave at subwavelength scale. From the dispersion relation of surface mode, an explicit expression can be obtained to map the effective refractive index into the hole depth of the unit cell. Arbitrary GRIN profile with effective refractive index higher than that of air can thus be straightforwardly implemented by simply adjusting the spatial distribution of the hole depth. Our work provides a feasible pathway to the subwavelength manipulation of airborne sound as well as an ideal experimental platform to directly observe the wave propagation and energy flow inside GRIN media.

Uncertainty Propagation in Thermo-mechanical Behaviors of Functionally Graded Plates Existing Unknown-but-Bounded Parameters

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ABSTRACT

Functionally graded (FG) materials, which are composed of two or more phases with different material properties, offer excellent performance in high-temperature environment. However, due to the limitations of technology and operation condition, the errors of manufacturing and processing lead to the uncertainty in material properties. The deterministic analyses are insufficient to provide a complete prediction of the structural response. Therefore, it is indispensable to develop uncertainty propagation model to reflect the effects of uncertain material properties on the mechanical behaviors of functionally graded structures. This presentation focuses on the effects of the uncertainty in material properties on the free vibration characteristics of rectangular FG plates in thermal environment. The deterministic model for thermo-mechanical behavior is presented in the framework of classic thin plate theory. Then a non-deterministic model for the free vibration of rectangular FG plates, in which temperature effect and uncertain material properties are considered, is developed. For probabilistic methods, sufficient information about the uncertainty is often impossible or very expensive to obtain to define the precise probability distributions. Meanwhile, even small variations from real values may result in large errors in probability distributions of the design space. In order to overcome the demerits of probabilistic approach in the case of inadequate data, the material uncertainties are quantified as interval variables. Based on the set theory, an interval iterative method (IIM) for solving this model is proposed to seek the bounds of uncertain natural frequencies. Meanwhile, the Monte Carlo simulation (MCS) is employed as the referenced result to validate the accuracy and efficiency of the IIM. Subsequently, extensive investigations are performed to reveal the combined effects of the material uncertainties and power law index, aspect ratio, thickness to length ratio as well as temperature change on the natural frequencies. Finally, some conclusions are summarized, which are meaningful in practical engineering applications to realize a safe and reliable design.

A Background Mesh Approach to Fluid-Structure Interaction Using PFEM

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ABSTRACT

Both fixed and moving finite element (FE) mesh can be used with Lagrangian based fluid analysis (Idelsohn et al 2013). Although the fixed mesh is always of good computational quality, it is difficult to be extended to fluid-structure interaction (FSI). As in Becker et al (2015), the structural domain with the hypoelastic model is simulated with a fluid-like formulation in order to use the fixed mesh for the structures. However, arbitrary structural types, such as beams and columns, cannot always be modeled with a fixed mesh. On the other hand, the moving mesh is flexible for any structural type and simulating the complex interaction between fluid and structure, but the quality and size of elements are difficult to control due to the random locations of fluid particles. The background mesh approach combines the advantages of both methods, using a fixed mesh for the fluid only domain and a moving mesh for the FSI domain. Massless fluid particles transport fluid properties over the fixed mesh as in Becker et al (2015). The problem with the fixed mesh for FSI is the arbitrary locations of structural nodes which can be very close to the fixed nodes of the fixed mesh when the structure undergoes large displacements. To resolve this problem, when fluid particles enter the FSI domain, the fixed nodes that are close to structural nodes are removed and the Delaunay Triangulation is used to generate a moving mesh between the remaining fixed nodes and structural nodes. As a result, the majority of the fluid domain uses the good quality fixed mesh and the moving FSI mesh is flexible for different structural types. The current fully Lagrangian FSI solvers (Zhu and Scott 2014) for the particle finite element method (PFEM) can be used without modification and its efficiency is increased with the partial fixed mesh. Becker, P., Idelsohn, S., and Oñate, E. (2015). "A unified monolithic approach for multi-fluid flows and fluid-structure interaction using the particle finite element method with fixed mesh." *Computational Mechanics*, 55(6), 1091–1104. Idelsohn, S. R., Nigro, N. M., Gimenez, J. M., Rossi, R., and Marti, J. M. (2013). "A fast and accurate method to solve the incompressible Navier-Stokes equations." *Engineering Computations*, 30(2), 197–222. Zhu, M. and Scott, M. H. (2014). "Improved fractional step method for simulating fluid-structure interaction using the PFEM." *International Journal for Numerical Methods in Engineering*, 99(12), 925–944.

Integrating Computational Modeling with in situ TEM for Understanding the Degradation in Lithium-ion Battery Electrodes

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ABSTRACT

Lithium-ion batteries play a pivotal role in the emerging renewable energy landscape. However, they suffer from the electrochemically-induced mechanical degradation in high-capacity electrodes, resulting in fast capacity fade and short cycle life. We have developed a unique nanoscale battery cell inside transmission electron microscope (TEM), which enables the real-time observations of reaction, deformation and degradation in individual nanowire and nanoparticle electrodes. In this talk, I will present our recent studies that integrate computational modeling with in situ TEM for understanding the degradation in Lithium-ion battery electrodes. Examples include the lithiation of Si nanowires with different types of coatings, delithiation of Ge nanoparticles, and lithiation of composite Si/Ge nanowire electrodes. Our results provide new insights into the microstructural evolution and mechanical degradation in battery electrodes, and have broad implications for designing the durable electrodes in high-performance rechargeable batteries.

B++ Splines with Applications in XIGA, Topology Optimization and Sheet Metal Forming

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ABSTRACT

In the fields of XIGA, topology optimization and IGA-based sheet metal forming for trimmed CAD geometries, imposing strong Dirichlet boundary conditions on the complex geometric boundaries is still a challenge. In this paper, we will introduce recent researches in the fields of XIGA, topology optimization and sheet metal forming using B++ splines. B++ splines mean "Boundary Plus Plus Splines". B++ Splines can integrate the boundary description and background meshes into a unity representation which allows imposing strong Dirichlet boundary conditions. We have developed bivariate B++ splines for trimmed NURBS surfaces [1] and trivariate B++ splines for B-rep models respectively. Recently, we applied B++ Splines to the fields of XIGA, topology optimization and sheet metal forming. First, we proposed XIGA based on B++ splines. Compared with traditional XIGA, the presented method allows imposing strong Dirichlet boundary conditions in the weak or strong discontinuous interfaces. Second, we developed a topology optimization method using B++ splines. Compared with traditional topology optimization methods using Heaviside functions, our method does not rely on Heaviside functions and simplifies the analysis procedure significantly. Third, inspired by the pioneering work by Benson et al. [2] in sheet metal forming, we developed an initial solution estimation algorithm [3] for One-step inverse IGA and B++ spline-based isogeometric shell analysis of trimmed CAD surfaces, which are expected to be applied into the simulations of sheet metal forming. The aforementioned researches imply that B++ splines have a wide range of applications in the field of isogeometric analysis, especially for the simulation of the engineering problems with complex geometric boundaries. [1] Zhu, X., Hu, P., & Ma, Z. D. (2016). B++ splines with applications to isogeometric analysis. *Computer Methods in Applied Mechanics and Engineering*, 311, 503-536. [2] Benson, D. J., Bazilevs, Y., Hsu, M. C., & Hughes, T. J. R. (2011). A large deformation, rotation-free, isogeometric shell. *Computer Methods in Applied Mechanics and Engineering*, 200(13), 1367-1378. [3] Zhang, X., Zhu, X.*, Wang, C., Liu, H., Zhou, Y., Gai, Y., ... & Ma, Z. D. (2018). Initial solution estimation for one-step inverse isogeometric analysis in sheet metal stamping. *Computer Methods in Applied Mechanics and Engineering*, 330, 629-645.

A Multi-Fidelity Stochastic Collocation Method for Time-Dependent Problems

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ABSTRACT

In this talk, we shall discuss a collocation method with multi-fidelity simulation models to efficiently reconstruct the time trajectory of time-dependent parameterized problems. By utilizing the time trajectories of low/high-fidelity solutions to construct the approximation space, this method is demonstrated to offer two substantial advantages: (1) it is able to produce more accurate results with a limited number of high-fidelity simulations; (2) it avoids instability issues of time-dependent problems due to the nonintrusive nature. We also provide several numerical examples to illustrate the effectiveness and applicability of the method.

Study of Fish Self-adapting Behaviour in Karman Vortex Street Using Reinforcement Learning

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ABSTRACT

Rocks and other objects in the flow can generate a repeating pattern of swirling vortices, known as the Karman vortex street. Fish (like rainbow trout) in these vortices show a large-amplitude lateral motion of the body occurring at a low frequency, to achieve high efficient swimming (Stewart et al., 2016). This behaviour involves two essential processes: sensing the ambient flow using the lateral line (Liao, 2006) and dynamically adjusting swimming pattern to maximize the performance in respond to the flow. However, it is still unclear how fish achieve these complex processes. What flow information is really useful in this process? How the fish respond to the information? What is the basic flow mechanism behind it? In this work, we intend to gain a deeper understanding of these questions by building a numerical model of a fish to optimize its performance in a Karman vortex street. This is achieved by combining an immersed boundary--lattice-Boltzmann method (IB-LBM) and the reinforcement learning algorithm. The IB-LBM is employed to calculate the flow dynamics caused by a fish-like foil movement due to its simplicity and high efficiency. The foil is put in a vortex street generated by a cylinder in a uniform stream. The foil employs a reinforcement learning algorithm to alter its swimming kinematics. The algorithm tries different swimming amplitudes and frequencies (states, actions) and observes the change in flow velocity and pressure in the ambient flow (rewards). By analysing these states, actions and rewards, the fish automatically finds a way to achieve optimal performance with a sequence of actions in different states. To the best of our knowledge, this work is the first attempt to simulate the fish self-adapting behaviour in a Karman vortex street including both the flow sensing and feedback control processes. It will provide deeper understanding of this behaviour and benefit the design of maneuverable autonomous underwater vehicles. Liao, J. C. (2006). The role of the lateral line and vision on body kinematics and hydrodynamic preference of rainbow trout in turbulent flow. *Journal of Experimental Biology*, 209(20), 4077-4090. Stewart, W. J., Tian, F. B., Akanyeti, O., Walker, C. J., &&&&& Liao, J. C. (2016). Refuging rainbow trout selectively exploit flows behind tandem cylinders. *Journal of Experimental Biology*, 219(14), 2182-2191.

Homogenisation of Dislocation System and Dislocation Pattern Formation

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ABSTRACT

Proper formulation of multiple-scale dislocation interactions is crucial for continuum model of dislocation to capture the various types of dislocation patterns formed in crystalline materials. In this talk, starting with discussion on homogenising the behaviour of a row of dislocation dipoles, we will show by matched asymptotic expansion that discrete dislocation dynamics (DDD) can be effectively upscaled by a set of evolution equations for dislocation densities along with a set of equilibrium equations for variables characterising the self-locked dislocation structures (SLDSs) which can be treated quasi-steadily on the continuum scale. The stress to unlock the SLDSs, i.e. the flow stress, can be determined by checking the solvability conditions of the local equations that govern the steady state of SLDSs. Based on these findings, a general strategy of summarising the collective behaviour of many dislocations will be presented. Under this guideline, a (continuum) flow stress formula for multi-slip systems, which resolves more details from the underlying dynamics than the ubiquitously adopted Taylor-type formulae, is derived. Moreover, the continuum dynamics of the formation, migration and dissociation of SLDSs on parallel slip planes can be successfully formulated in good accordance with the underlying DDD.

Numerical Simulation of PMMA Foaming Process Assisted by Supercritical Carbon Dioxide: Bubble Growth Dynamics

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ABSTRACT

In this paper, the bubble growth process of PMMA/supercritical carbon dioxide system in an isothermal condition was simulated. Based on the cell model, a mathematical model for bubble growth was established by solving the continuity equation, momentum equation, mass equation, diffusion equation and constitutive equation. Through the numerical simulation of MATLAB, the effects of process parameters on bubble growth were investigated. The results show that the foaming temperature and the saturation pressure significantly affect the cell growth process, in which the foaming temperature significantly affects the viscosity of the matrix, the nucleation rate of the cell, the amount of carbon dioxide adsorbed and the diffusion rate to the cell. The saturation pressure significantly affects the nucleation rate and the amount of carbon dioxide absorption. The simulation results prove that with the foaming temperature increasing, the size of bubble increases exponentially and the bubble size decreases linearly with the increasing of saturation pressure. The numerical simulation results in this paper have significant guidance on the foaming process.

Theoretical and Numerical Models to Predict and Optimize Fracking in Shale

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ABSTRACT

Hydraulic fracture (fracking) technology in gas or oil shale field engineering is highly developed last decades in North America and also recent years in China, but the knowledge of actual fracturing process is mostly empirical and makes a mechanician wonder: Why the fracking works? In this work, the theoretical and numerical models to predict and optimize fracking are proposed for fracking simulation in shale rock. The first work is fracking prediction. The self-consistent fracture condition based on extended finite element method (XFEM) is resulting in fluid flux, perforation entry loss and energy release rate to drive multi-scale fracture growth or arrest. However, there are million smeared fractures in the horizontal perforation wellbore, which is beyond computation capacity. XFEM is only suitable for major fractures, so the multi-scale self-consistent model of damage volume ratio is developed to predict pressured fluid flow in wellbore and global production in field engineering from the stimulated reservoir volume (SRV) based on the required fracture spacing order, reservoir pressure and proppant size, as well as the other given conditions. Some examples are provided to test and verify the models. The second work is fracking optimization. Shale is a typical layered and anisotropic material whose properties are characterized primarily by locally oriented anisotropic clay minerals and naturally formed bedding planes. The debonding of bedding planes will greatly influence the shale fracking to form a large-scale highly permeable fracture network, named SRV. Both theoretical and numerical models are developed to quantitatively predict the growth of debonding zone in layered shale under fracking, and the good agreement is obtained between the theoretical and numerical prediction results. Some parameters are proposed to characterize the corresponding conditions of tensile and shear debonding of bedding planes. It is found that debonding is mainly caused by the shear failure of bedding planes in the actual reservoir. Then the theoretical model is applied to design the perforation cluster spacing to optimize SRV, which is a critical issue in fracking. If the spacing is too small, there are overlapping areas of SRV and the fracking efficiency is much lower. If the spacing is too large, some strata can't be stimulated. Simultaneously, the parameters of SRV and efficiency are proposed. Through maximizing the values of these parameters, the SRV and optimal perforation cluster spacing range can be quantitatively calculated to guide the fracking treatment design. These results are comparable with the data from field engineering. Keywords: Hydraulic fracture, Stimulate reservoir volume, Theoretical and numerical models, Fracking prediction and optimization, Shale rock

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The Strategy for Modeling and Solving Uncertainly Defined Boundary Value Problems

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ABSTRACT

Solving different types of problems most often leads to solving different types of partial differential equations. As it is known from the literature, they can be elliptic, parabolic or hyperbolic type. The great variety of these equations gives many possibilities for modeling and solving various practical problems. To solve them, numerical methods are used, among which the finite and boundary element methods or meshless methods should be mentioned. A common feature of all mentioned differential equations and the methods of solving them is that their physical definition requires input data determined in a precise manner, i.e. the shape of the boundary, boundary conditions and other parameters are given in the form of exact numerical values. This is some idealization of reality, because these data are measured, and hence contains errors related to the inaccuracy of a measuring device. To take into account all these inaccuracies, an effective strategy for comprehensive modeling of uncertainty of the boundary problem should be developed. In the literature some preliminary papers are presented allowing for a consideration of the uncertainty of the system's parameters or boundary conditions. However, there are no papers about the uncertainly defined shapes or papers comprehensively considering all the above-mentioned uncertainties. The main aim of the research is to develop a comprehensive modeling strategy for these uncertainties, as well as a method for solving such defined problems. For this purpose, the parametric integral equation system (PIES) previously developed by one of the co-authors and successfully used to solve various precisely defined problems should be generalized [1]. It consists in the assumption that the input data are defined using interval arithmetic. Therefore, it must be included everywhere in the PIES mathematical apparatus by appropriate modifications. However, after many tests, it was decided to use the directed interval arithmetic, not classical one. Nevertheless, even this arithmetic has to be modified in order to properly model uncertainty. Such modified arithmetic was also applied for numerical solution of interval PIES. The paper presents examples of modeling and solving uncertainly defined potential boundary value problems using the proposed strategy. References: [1] Zieniuk E., Sawicki D., Boltuc A.: Parametric integral equations systems in 2D transient heat conduction analysis, *Int. J. Heat Mass Transf.*, 78 (2014), s. 571 – 587.

The Effect of Cavitation on the Temperature Elevation during Focused Ultrasound Therapy

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ABSTRACT

The present study investigates the cavitation presence impact on the HIFU thermal therapy process in soft tissue. The key aspects have been covered: dependency of the bubble dynamics on soft tissue viscoelastic properties, temperature elevation inside and outside the bubble, bubble-bubble interaction and corresponding to it translational motion of the bubbles, the comparison with real experiments. For the mentioned purposes, new coupled models have been proposed, describing bubble dynamics with Gilmore-Akulichev model, soft tissue with Zener viscoelastic model, temperature elevation with interrelated heat equations for bubble's interior and exterior. Bubble-bubble interaction was modeled using Doinikov's model. The comparison with experiments has been performed on the basis of the predicted temperature elevation in a soft tissue with cavitations effect taken into account.

A Finite Element Algorithm for Large Deformation Frictional Contact of Multiphasic Materials with Multiple Neutral and Charged Solutes

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ABSTRACT

Contact of multiphasic soft tissues is an important topic in biomechanics, particularly in understanding damage and failure mechanisms in diarthrodial joints, where opposing cartilage surfaces undergo reciprocal contact loading for thousands of cycles per day. Previous work [1] on injurious frictional loading of juvenile bovine cartilage has shown damage to collagen fibrils and the concomitant formation of a swollen blister, which forms due to mechanochemical interactions between ionic species in the interstitial fluid and charged molecules bound to the solid matrix. Capturing the salient characteristics of this damage cascade in a computational framework necessitates multiphysics modeling of these solutes, and their interactions with the charged solid matrix, under frictional contact conditions. To date, however, finite element algorithms for multiphasic contact are restricted to frictionless conditions, precluding the simulation of friction-mediated processes. FEBio is a free finite element software package designed to meet the computational needs of the biomechanics and biophysics community (febio.org) [2]. This study describes the formulation of a novel finite element algorithm for frictional contact of multiphasic materials and its implementation and verification in FEBio. Previously [3] we developed a finite element algorithm for frictional contact of biphasic materials that coupled interstitial fluid pressurization to the frictional response. The extension to multiphasic contact is more challenging, as it requires coupling of chemical and osmotic interactions with the mechanical and fluid pressurization response, and has yet to be achieved. We propose to overcome these challenges by implementing our model of multiphasic friction in a large deformation finite element algorithm that relates the frictional traction to the effective fluid pressure inside the tissue. In a multiphasic analysis, it is well known that fluid pressures are not continuous and thus cannot be used as nodal variables. However, the effective fluid pressure, which is inclusive of osmotic effects, is continuous and thus may be used as a nodal variable. In this framework, the frictional traction in a multiphasic material is proportional only to the fraction of normal traction transmitted via solid-solid interactions across the contact interface. Consequently, an elevated effective fluid pressure, whether due to osmotic or mechanical effects, will reduce the friction coefficient, achieving the desired mechanochemical coupling. The model is validated against our experimental investigations of osmotic pressure-driven frictional behavior, successfully demonstrating unique behaviors previously unobtainable by finite element methods. References [1] Durney, KM+, SB3C 1071, 2016 [2] Maas, S+, J Biomech Eng, 2012 [3] Zimmerman, BK+, SB3C 179, 2017

Assessing the Fracture Strength of Geological and Related Materials in Fluid Environments via an Atomistically Based J-integral

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ABSTRACT

Predicting fracture initiation and propagation in low-permeability geomaterials is a critical yet unsolved problem crucial to assessing shale caprocks at carbon dioxide sequestration sites, and controlling fracturing for gas and oil extraction. Experiments indicate that chemical reactions at fluid-geomaterial interfaces play a major role in subcritical crack growth by weakening the material and altering crack nucleation and growth rates. Engineering the subsurface fracture environment, however, has been hindered by a lack of understanding of the mechanisms relating chemical environment to mechanical outcome, and a lack of capability directly linking atomistic insight to macroscale observables. We have developed a fundamental atomic-level understanding of the chemical-mechanical mechanisms that control subcritical cracks through coarse-graining data from reactive molecular simulations. Previous studies of fracture at the atomic level have typically been limited to producing stress-strain curves, quantifying either the system-level stress or energy at which fracture propagation occurs. As such, these curves are neither characteristic of nor insightful regarding fracture features local to the crack tip. In contrast, configurational forces, such as the J-integral, are specific to the crack in that they measure the energy available to move the crack and truly quantify fracture resistance. By development and use of field estimators consistent with the continuum conservation properties we are able to connect the data produced by atomistic simulation to the continuum-level theory of fracture mechanics and thus inform engineering decisions. In order to trust this connection we have performed theoretical consistency tests and validation with experimental data. Although we have targeted geomaterials, this capability can have direct impact on other unsolved technological problems such as predicting the corrosion and embrittlement of metals and ceramics. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525

Role of Bone's Multi-scale Structure in Resisting Deformation and Fracture

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ABSTRACT

Bone is an extremely tough and yet lightweight material that provides structural support to organisms. In this context, bone provides mechanical resistance to physiological forces with the additional capacity for self-repair and adaptation to changing loading environments. Bone's mechanical resistance derives from its complex hierarchical structure, which spans from macroscopic length-scales including bone's macro-architecture to the nanometer scale, consisting of collagen molecules and mineral platelets. Specifically, bone's strength and ductility originate primarily at the nano to submicrometer structure through deformation of its mineralized collagen fibrils. Bone toughness (i.e., resistance to crack initiation and growth) is generated at much larger, micro- to near-millimeter, scales from crack-tip shielding associated with interactions between the crack path and the microstructure. Here, we discuss how these multi-scale deformation and toughening mechanisms resist fracture in more complex physiological loading conditions. For instance, in high strain rate conditions, time-dependent, viscous mechanical component is suppressed, which affects the tissue's capacity for fibrillar sliding and crack deflection mechanisms that generate toughness at lower strain rates. Furthermore, we discuss how fracture resistance becomes degraded in biological aging and disease conditions, leading to increased risk of fracture. The aging- and disease-related change in mechanical properties stems from alterations to the structural features at multiple length-scales, including the collagen cross-linking environment, the homogeneity of mineralization, and the density of the osteonal structures. Studying the origins of bone's fracture resistance in physiological and disease conditions aids further progress in the diagnosis, prevention, and treatment of diseases that increase the fracture risk or affect the mechanical integrity of human cortical bone.

Bridging the Gap between Domain Experts and Computer Scientists with Tiger Teams in the bwHPC-C5 Project

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ABSTRACT

The Coordinated Compute Cluster Competence Centers ("bwHPC-C5") are a state-funded project with the participation of eleven universities, which offers federated support for users of six High Performance Computing (HPC) clusters in the state of Baden-Württemberg, Germany. Users of these HPC systems can request "Tiger Teams", which are formed by the users (domain experts) as well as members of the computing centers (computer scientists). The work performed in the Tiger Teams includes advising users for optimal usage of HPC systems, porting code to other clusters, parallelization of sequential parts of code and optimization of data management as well as performance of user applications. One example of a Tiger Team from the "Competence Center Engineering" is given by a user, whose application requires a lot of memory per process due to a complex particle tracking code that is coupled to the open-source CFD code OpenFOAM. In a Tiger Team, the user's application was ported to the "JUSTUS" cluster, which has been specifically designed for quantum chemistry codes and thus has more memory per node. Besides the work of the Tiger Teams, we also present an example for performance optimization of a CFD code for combustion processes. The code is a coupling between OpenFOAM and the open-source chemistry library Cantera. A large part of total simulation time was spent on computing chemical reaction rates. The user provides a text file which contains the set of chemical reactions. This text file is read at the start of the simulation and used to compute the chemical reaction rates during simulation. In order to speed this up, a converter tool was developed which automatically converts the text file into C++ source code. The code contains all routines needed for computing the chemical reaction rates and is generated in a way that makes it easy for the compiler to perform optimizations. For example, the data is laid out in a way that loops can easily be auto-vectorized, which will become more important on future architectures. Due to OpenFOAM's runtime selection mechanism, the user can quickly modify the simulation setup to incorporate the new routines. By using the optimized routines, total simulation time could be reduced by 40%. In addition to these serial optimizations, parallel performance analysis tools like ScoreP/Vampir and Extrae/Paraver have been applied in order to improve load balancing. The optimized application shows nearly ideal speedup and has been run on up to 28,800 CPU cores.

An XFEM/DG Method for the Simulation of Valve Dynamics through a Fluid-Structure Interaction Problem

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ABSTRACT

We present an unfitted numerical method for the simulation of fluid-structure interaction (FSI) problems in the case of an incompressible fluid that interacts with an immersed elastic structure. In particular, we consider a full three-dimensional model for the structure, though its thickness is smaller than its characteristic size. We apply this strategy to the simulation of heart valves dynamics. The proposed method is based on the eXtended Finite Element Method (XFEM) which relies on unfitted and overlapping meshes, in particular the structure mesh overlaps the fluid one. The advantage of this approach is that the structure mesh is allowed to move independently of the fluid (background) one, which is fixed. As result, the fluid-structure interface intersects the background elements in an arbitrary configuration. This generates cut-elements of generic (polyhedral) shape that require a special treatment for integration and accuracy purposes. The coupling between the fluid and structure problems is taken into account by means of a Discontinuous Galerkin (DG) mortar applied to the fluid-structure interface. We present several 3D numerical results featuring realistic Reynolds numbers that highlight the suitability of the proposed method.

Field-aligned Parametrization and Quad Layout Construction

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ABSTRACT

A variety of techniques were proposed to model smooth surfaces of arbitrary topology based on tensor product splines (e.g. subdivision surfaces, free-form splines, T-splines). Conversion of an input surface into such a representation is commonly achieved by constructing a global seamless parametrization, possibly aligned to a guiding cross-field and using this parametrization as a domain to construct the spline-based surface. (Informally, seamless parametrizations can be thought of as parametrizations of surfaces cut to disks, with isoparametric line directions and spacing on the surface matching perfectly across the cuts). A quad layout can be constructed from such parametrizations. One major fundamental difficulty in designing robust algorithms for this task is the fact that for common types, e.g. that spline surfaces or subdivision surfaces, reliably obtaining a suitable parametrization that has the same topological structure as the guiding field, in particular, having exactly the same singularities, poses a major challenge. Even worse, not all fields admit compatible parametrizations: in some cases, singularities need to be added, or the field modified in other ways. In other words, it is not known for what singularity choices defined by the user or automatically, there is a matching spline layout. I will discuss our recent work that addresses the problem. In particular, I will present a complete solution based on the new concept of seamless similarity maps (a relaxation of the seamless parametrization definition, allowing scale jumps across cuts) and a matching spline construction. It turns out, that for any given guiding field structure, a compatible parametrization of this kind exists and can be computed by a relatively simple algorithm; at the same time, for any such parametrization, a smooth piecewise rational surface with exactly the same structure as the input field can be constructed from it. Further I will discuss a solution that imposes more restrictive requirements (but still allows essentially arbitrary singularity configurations) but does not require using similarity maps. Both of these approaches lead to fully automatic construction of high-order approximations of arbitrary surfaces, even with highly complex topology, potentially enabling, e.g., robust automatic conversion of surfaces to isogeometric form.

Experiments, Continuous and Discrete Simulations of the Role of an Inclined Bottom on the Lateral Discharge Flow of Granular Media from Silos

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ABSTRACT

In the context of safety studies of nuclear power plants, we consider an hypothetical scenario of a control rod ejection leading to a reactivity insertion. During such an accident, the cladding of the fuel rods is severely stressed and standard safety studies ensure its integrity. In this study, we go beyond this statement and assume the failure of the cladding of some fuel rods. Fuel fragments and fission gas at high temperature could then be ejected toward the surrounding coolant and exchange rapidly a large amount of heat. The violence of this interaction depends particularly on the discharge flow rate of fragments toward the fluid. In the present work, we represent the fuel fragments as a dry granular media and the clad as a vertical reservoir, a silo. The ejection of fuel fragment is simulated by the discharge of the granular media through an orifice on one lateral side of the silo. We focus especially on the influence of the internal geometry of the reservoir on the discharge flow thanks to experiments, continuous and discrete numerical simulations. Continuous simulations are done thanks to an implementation of frictional rheology in a volume of fluid incompressible free code (Basilisk) which solves Navier-Stokes equations. Discrete simulations use the free solver LMGC90 implementation of the contact dynamic method. More precisely, the reservoir has an inclined bottom which ends up at the lateral orifice. The controlled parameters are the height of the orifice D , the thickness of the silo W , the bottom inclination angle and the particles size. The measured parameters are the mass flow rate and the velocity field near the orifice, obtained thanks to Particle Image Velocimetry. We have compared laboratory experiments, continuous and discrete numerical simulations and observed an excellent agreement between experimental and simulation results. We found that the grains velocity at the center of the orifice only depends on its size. Two granular flow regimes have been identified. The first regime is observed for small inclination of the bottom : the granular flow orientation is controlled by the aspect ratio D/W , the higher D/W , the more the flow is aligned with gravity. The second regime is observed for large inclination of the bottom : the flow orientation is strongly correlated with the angle. Finally, we present a model that predicts the discharge flow rate of particles from a rectangular silo with an inclined bottom according to its aspect ratio.

Applying Isogeometric Shells to Unstructured U-spline Surfaces

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ABSTRACT

In this talk we will describe our efforts to extend the isogeometric Kirchhoff-Love and geometrically exact Reissner-Mindlin shells to a newly developed spline representation called U-splines. A U-spline surface allows unstructured meshes and overcomes the analysis-suitability restrictions of a T-spline while preserving the mathematical properties required by analysis. This enables us to apply isogeometric shell formulations to complex engineering structures. We also explore the imposition of C1 continuity constraints around the extraordinary points in U-spline, which makes the higher order isogeometric shells applicable to complex meshes with extraordinary points. We demonstrate the effectiveness of the approach on several carefully selected numerical benchmarks.

On a New Mixed Formulation of Kirchhoff and Reissner-Mindlin Plates

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ABSTRACT

In 3D linear elasticity it is well-known that stress tensor fields satisfying the homogeneous equilibrium equation can be expressed in terms of the Beltrami stress functions provided the domain is topologically simple. There is a similar result for the tensor field of bending and twisting moments in plate models, if the mid-surface of the plate is simply connected. While the stress tensor field in 3D linear elasticity can be written as a second-order differential operator applied to the Beltrami stress functions, the tensor field of bending and twisting moments in plate models is only a first-order differential operator applied to some 2D vector field. We will show how this result can be used to reformulate the Kirchhoff and the Reissner-Mindlin plate models as well-posed second-order systems. The incorporation of mixed boundary conditions describing clamped, simply supported, and free parts of the plate's boundary as well as corner conditions are discussed. For the Kirchhoff model the second-order system consists of three (consecutively to solve) standard second-order elliptic problems, see [1,2]. For the Reissner-Mindlin model the ideas from [1,2] are combined with the formulation in [3] (presented there, more generally, for shells) and result in two second-order elliptic problems and one saddle point problem. The reformulation of the plate models as second-order systems allows for discretization methods in approximation spaces with continuous functions. This includes standard continuous Lagrangian finite element methods and spline spaces from isogeometric analysis on multi-patch domains with continuous patching only. [1] W. Krendl, K. Rafetseder, and W. Zulehner. A decomposition result for biharmonic problems and the Hellan-Herrmann-Johnson method, ETNA, Electron. Trans. Numer. Anal., 45, pp. 257–282, 2016. [2] K. Rafetseder and W. Zulehner. A decomposition result for Kirchhoff plate bending problems and a new discretization approach. ArXiv e-prints, arXiv:1703.07962, pp. 1-27, March 2017. [3] R. Echter, B. Oesterle and M. Bischoff. A hierarchic family of isogeometric shell finite elements, Comput. Methods Appl. Mech. Engrg., 254, pp. 170–180, 2013.

A Fictitious Domain Method for Fluid-Structure Interaction

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ABSTRACT

We present a new and completely parallel approach for fluid-structure interaction with contact between the elastic structures. Our approach is inspired by the fictitious domain method [1] and exploits variational transfer techniques for coupling the solid and the fluid and on the possibly contacting surfaces between solids [2]. The main idea of the fictitious domain method is modeling the solid phase as immersed in a background fluid phase. The fluid is described in an Eulerian fashion (fixed mesh), while we use Lagrangian meshes for the solid structure. The coupling between the two phases is achieved with overlapping domain decomposition. Specifically, our coupling is constructed by means of L2-projections where a Lagrange multiplier is used to weakly enforce the velocity vector constraint along the interface-boundary between the solid and the fluid. For solving the arising nonlinear-system of discrete equations we adopt a staggered approach within a fixed-point iteration, hence the fluid and the solid problems are solved separately with the following four steps: First, we transfer velocities from the solid mesh to the fluid mesh. Second, we solve the fluid dynamics problem by imposing the velocity constraint in the overlapping region. Third, we compute and transfer the reaction force from the fluid mesh to the boundary of the solid mesh. At last, we solve the solid mechanics problem by imposing the reaction force on the solid (Neumann) boundary. We present the discretization, the setup of the parallel variational transfer [3], methods for the solution of the arising non-linear problems, and the related software libraries we developed. We present 2D and 3D benchmarks, and a tricuspid heart valve. [1] F. P. Baaijens. A fictitious domain/mortar element method for fluid-structure interaction. *International Journal for Numerical Methods in Fluids*, 35(7):743–761, 2001. [2] T. Dickopf and R. Krause. Efficient simulation of multi-body contact problems on complex geometries: A flexible decomposition approach using constrained minimization. *International journal for numerical methods in engineering*, 77(13):1834–1862, 2009. [3] R. Krause and P. Zulian. A parallel approach to the variational transfer of discrete fields between arbitrarily distributed unstructured finite element meshes. *SIAM Journal on Scientific Computing*, 38(3):C307–C333, 2016.

ADVANTAGES OF AUTOMATIC-DIFFERENTIATION-BASED FORMULATION AND SENSITIVITY ANALYSIS BASED IMPLEMENTATION OF MULTISCALE METHODS

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Key words: Multiscale methods, MIEL, FE^2 , sensitivity analysis, path dependent problems, convergence

Summary. Multiscale methods became a strong field in computational mechanics, partly because of a need for detailed analysis of response with respect to material and geometric nonlinearities and thanks to growing computer capabilities. In this paper, focus is on advantages of Automatic-Differentiation-Based formulation and sensitivity analysis based implementation, especially convergence rate of two frequently used multiscale methods, MIEL and FE^2 . Their implementation is carried out with AceGen and AceFEM based on analytical sensitivity analysis and is compared to Schur complement based one. Sensitivity analysis based implementation assures efficient and consistent multiscale modeling. It is shown that quadratic convergence is achieved also for path dependent problems with two interacting continuation methods.

1 INTRODUCTION

Multiscale methods are growing trend in computational mechanics, especially with increasing capabilities of computers. Many of the multiscale methods originate from the demand to model heterogeneous materials [1]. Roughly, multiscale methods can be divided into two groups: methods that are based on homogenization techniques and domain decomposition methods. For purpose of convergence comparison, one method from each group was implemented, FE^2 and MIEL. Numerical schemes for implementation

of MIEL and FE² multiscale methods, based on sensitivity analysis and with use of Schur complement, are presented. Implementation is done with the Mathematica packages AceGen and AceFEM [2]. These programs enable analytical sensitivity analysis of first and second order, which can be used for efficient implementation of multiscale finite element methods. Computational environment was created, where the multiscale program code is automatically derived and various types of multiscale and single scale approaches can be freely mixed, while retaining quadratic convergence of the two-level Newton-Raphson procedure.

2 AUTOMATION OF PRIMAL AND SENSITIVITY ANALYSIS

The AceGen is an advanced automatic code generator, where automatic differentiation technique, automatic code optimization and generation are combined with computer algebra system Mathematica [3]. The AceFEM package is a general finite element environment designed to solve multi-physics and multi-field problems. Automation of primal and sensitivity analysis is done with AceGen. The automatic differentiation technique (AD) can be used for the evaluation of the exact derivatives of any arbitrary complex function via chain rule and represents an alternative solution to the numerical differentiation and symbolic differentiation. The result of AD procedure is called "computational derivative" [4].

For automation of multiscale analysis the automation of primal analysis as well as first and second order sensitivity analysis are needed. In primal analysis the response of the system is evaluated, whereas in sensitivity analysis the derivatives of the response, e.g. displacements, strains, stresses or work, with respect to arbitrary design parameter ϕ_i are sought. The primal problem is solved by the standard Newton-Raphson iterative procedure (see e.g. [5]). For the automation of the multiscale methods the sensitivity analysis with respect to prescribed essential boundary conditions is needed.

For the path independent problems, the primal problem is defined with the residual equation $\mathbf{R}(\mathbf{p}) = \mathbf{0}$, where \mathbf{p} represents a set of nodal unknowns of the problem. For the boundary condition sensitivity analysis we define the residuals and the vectors of unknown as a function of a vector of design parameters $\boldsymbol{\phi}$ by

$$\mathbf{R}(\mathbf{p}(\boldsymbol{\phi}), \bar{\mathbf{p}}(\boldsymbol{\phi})) = \mathbf{0} \quad (1)$$

where $\bar{\mathbf{p}}$ represents a set of nodal unknowns with prescribed essential boundary conditions.

The sensitivity problem can be obtained from the primal problem by differentiating (1) with respect to design parameters (2). Equation (2) represents a system of linear equations (4) for the unknown sensitivities of the primal unknowns of the problem $\frac{D\mathbf{p}}{D\phi_i}$. The right hand side is called "first order sensitivity pseudo load vector". The vector $\frac{D\bar{\mathbf{p}}}{D\phi_i}$ represents the rate of the change of the prescribed essential boundary conditions, with respect to the change of design parameter and is called "prescribed boundary condition velocity field".

The sensitivity problem is solved after the convergence of the primal problem has been reached. For the automation we need only the ADB form (see [5]) of pseudo load vector ${}^I\tilde{\mathbf{R}}$ evaluated at the integration point of the individual finite element ${}^I\tilde{\mathbf{R}}_g$. The global pseudo load vector is then obtained by the standard integration over the element domain and the standard finite element assembly procedure of element contributions to global vector ${}^I\tilde{\mathbf{R}}_g$.

$$\frac{\partial \mathbf{R}}{\partial \mathbf{p}} \frac{D\mathbf{p}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \bar{\mathbf{p}}} \frac{D\bar{\mathbf{p}}}{D\phi_i} = \mathbf{0} \quad (2)$$

$${}^I\tilde{\mathbf{R}} = -\frac{\partial \mathbf{R}}{\partial \bar{\mathbf{p}}} \frac{D\bar{\mathbf{p}}}{D\phi_i} \quad (3)$$

$$\mathbf{K} \frac{D\mathbf{p}}{D\phi_i} = -{}^I\tilde{\mathbf{R}} \quad (4)$$

The second order sensitivity problem is obtained from the first order problem, by differentiating (2) with respect to design parameter ϕ_i . It results in

$$\begin{aligned} & \frac{\partial^2 \mathbf{R}}{\partial \mathbf{p}^2} \frac{D\mathbf{p}}{D\phi_i} \frac{D\mathbf{p}}{D\phi_j} + \frac{\partial^2 \mathbf{R}}{\partial \mathbf{p} \partial \bar{\mathbf{p}}} \frac{D\bar{\mathbf{p}}}{D\phi_j} \frac{D\mathbf{p}}{D\phi_i} + \frac{\partial \mathbf{R}}{\partial \mathbf{p}} \frac{D^2 \mathbf{p}}{D\phi_i D\phi_j} + \frac{\partial^2 \mathbf{R}}{\partial \bar{\mathbf{p}} \partial \mathbf{p}} \frac{D\mathbf{p}}{D\phi_j} \frac{D\bar{\mathbf{p}}}{D\phi_i} + \\ & + \frac{\partial^2 \mathbf{R}}{\partial \bar{\mathbf{p}}^2} \frac{D\bar{\mathbf{p}}}{D\phi_i} \frac{D\bar{\mathbf{p}}}{D\phi_j} + \frac{D\mathbf{R}}{D\bar{\mathbf{p}}} \frac{\partial^2 \bar{\mathbf{p}}}{\partial \phi_i \partial \phi_j} = \mathbf{0} \end{aligned} \quad (5)$$

$$\mathbf{K} \frac{D^2 \mathbf{p}}{D\phi_i D\phi_j} = -{}^{II}\tilde{\mathbf{R}} \quad (6)$$

where ${}^{II}\tilde{\mathbf{R}}$ represents the second order sensitivity pseudo load vector.

All first order sensitivities have to be calculated in order to be able to calculate the second order sensitivities. Equation (5) represents a system of linear equations (6) for the unknown sensitivities of the primal unknowns of the problem $\frac{D^2 \mathbf{p}}{D\phi_i D\phi_j}$. For ADB formulation (see [6]).

3 MULTISCALE METHODS

For overview of multiscale methods reader is referred to [7,8]. FE^2 is a standard two-level finite element homogenization approach [9], that is appropriate for the problems where scales are separated far enough and are only weakly coupled. In some cases, for example when difference between two scales is finite, or when in the region of high gradients, the FE^2 multi-scale approach fails, thus we need to use some sort of domain decomposition method. One possibility is the mesh-in-element or MIEL scheme described in [10].

3.1 FE^2 method

The FE^2 method is a two-level scheme, where we have one FE model for the macro scale (problem to be solved) and the second one at each material integration point (micro problem), as shown in Fig. 1. All information about micro-structure is obtained from

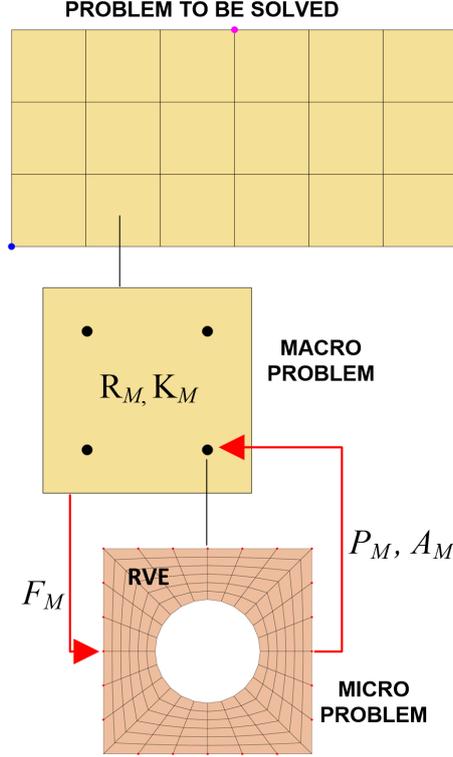


Figure 1: FE² procedure

computations on RVE-level by averaging the material response characterized by an appropriate stress measure and constitutive tangent matrix over RVE. RVE is attached to each integration point of the macroscopic FE problem. For a typical finite strain problem that leads to $\mathbf{P}_M = \{\mathbf{P}_m\}$ and $\mathbf{A}_M = \{\frac{\partial \mathbf{P}_m}{\partial \mathbf{F}_M}\}$, where \mathbf{P}_M and \mathbf{P}_m are the first Piola-Kirchoff stress tensors at macro and micro level, \mathbf{F}_M is the macroscopic deformation gradient and \mathbf{A}_M a macroscopic constitutive matrix. This information is then used at the macro level for the evaluation of integration point contribution to element residual \mathbf{R}_{Mg} and tangent matrix \mathbf{K}_{Mg} at the macro level, as follows

$$\mathbf{R}_{Mg} = \mathbf{P}_M : \frac{\partial \mathbf{F}_M}{\partial \mathbf{p}_{Me}} \quad (7)$$

$$\mathbf{K}_{Mg} = \frac{\partial \mathbf{R}_M}{\partial \mathbf{p}_{Me}} + \frac{\partial \mathbf{R}_M}{\partial \mathbf{P}_M} \mathbf{A}_M \frac{\partial \mathbf{F}_M}{\partial \mathbf{p}_{Me}} \quad (8)$$

where \mathbf{p}_{Me} represents a set of nodal unknowns of macro element. The FE² method can be implemented in different ways (see e.g. [9,11]). For efficiency of the method efficient calculation of the macroscopic constitutive matrix \mathbf{A}_M is important. In a conventional way of computing macroscopic constitutive tangent, computation of a Schur complement of RVEs tangent matrix is needed [9]. An alternative is calculation of consistent

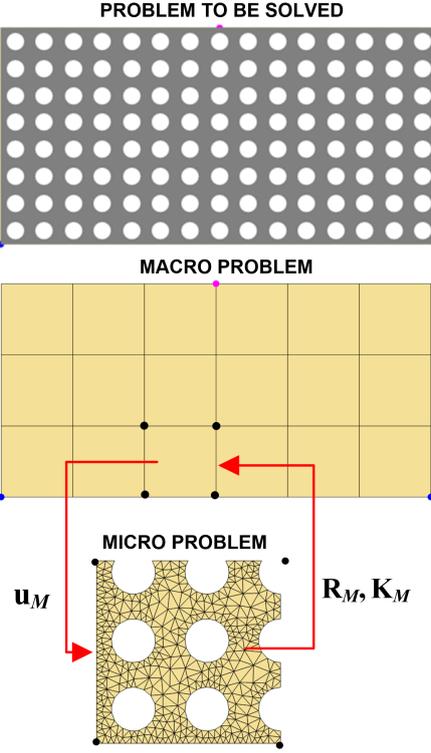


Figure 2: MIEL procedure

macroscopic stiffness matrix by sensitivity analysis of the micro-structure, with respect to macro strain measure used to impose boundary conditions on RVE. Sensitivity parameters of the problem are components of the macro deformation gradient \mathbf{F}_M , thus $\boldsymbol{\phi} = \{F_{M,11}, F_{M,12}, F_{M,13}, F_{M,21}, \dots\}$. For the complete formulation of the prescribed boundary condition sensitivity problem, prescribed boundary condition velocity field $\frac{D\bar{\mathbf{p}}}{D\boldsymbol{\phi}}$ is needed.

3.2 MIEL method

In case of MIEL the finite element models at different scales communicate between each other through degrees of freedom of the finite element at the macro scale. The residual and tangent matrix are for each macro element obtained directly from the micro scale problem. Each macro element thus represents one micro problem. MIEL procedure is presented in Fig. 2.

Macro tangent matrix is typically evaluated with the Schur complement of the global micro tangent matrix, thus elimination of inner DOFs. Here alternative implementation in AceFEM is presented, where macro tangent matrix is calculated through second order sensitivity analysis, with respect to prescribed essential boundary conditions. In that way, we get values of implicit dependencies of micro displacements on macro displacements.

Let \mathbf{p}_{Me} be a vector of unknowns in the nodes of the macro element, \mathbf{p}_{me} a vector of unknowns in the nodes of the characteristic micro problem element and W strain energy function. The outer shape of the micro problem is the same as the shape of the corresponding macro element. The prescribed essential boundary conditions (displacements) are identical to the displacements at the boundary of the corresponding macro element. The integration point contribution (g-th integration point in the e-th element of the micro mesh) to the macro residual and macro tangent matrix is then

$$\mathbf{R}_{Mg} = \frac{\partial W(\mathbf{p}_{me}(\mathbf{p}_{Me}))}{\partial \mathbf{p}_{Me}} = \frac{\partial W}{\partial \mathbf{p}_{me}} \frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}} \quad (9)$$

$$\mathbf{K}_{Mg} = \frac{\partial \mathbf{R}_{Mg}}{\partial \mathbf{p}_{Me}} = \frac{\partial^2 W}{\partial \mathbf{p}_{me}^2} \frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}} + \frac{\partial W}{\partial \mathbf{p}_{me}} \frac{D^2 \mathbf{p}_{me}}{D\mathbf{p}_{Me}^2}. \quad (10)$$

The implicit dependencies $\frac{D\mathbf{p}_{me}}{D\mathbf{p}_{Me}}$ and $\frac{D^2 \mathbf{p}_{me}}{D\mathbf{p}_{Me}^2}$ are obtained by the first and second order sensitivity analysis. Thus, the sensitivity analysis based automation of the MIEL scheme requires the second order sensitivity analysis for a set of sensitivity parameters \mathbf{p}_{Me} .

For the complete formulation of the prescribed boundary condition sensitivity problem, the first and the second order prescribed boundary condition velocity fields are needed, for details see e.g. [5] where the concept is extended to path dependent problems.

4 ADVANTAGES OF PROPOSED IMPLEMENTATION

In this section among other advantages improvement of convergence rate of implicit multiscale methods is presented, due to the automatic-differentiation-based formulation and sensitivity analysis based implementation, in comparison with Schur complement based implementation.

Solving of nonlinear problems is done implicitly with a two-level Newton-Raphson type iterative solution procedure. Here the macro path is parametrized by macro load level (λ_M). For every load step at macro level ($\Delta\lambda_M$), several substeps can be done at micro level ($\Delta\lambda_m$) where (λ_m) represents additional parameter at micro level used to parametrize micro problem within one macro load step. Since we have two scales, we have in general a path following procedure at both levels, resulting in two-level path following procedure presented in Fig. 3. Traditionally, each step at macro level is followed by only one step at micro level. Sensitivity analysis based multiscale analysis allows extension to more general case, where each macro step can be followed by an arbitrary number of micro substeps. For every substep at micro level, sensitivity has to be updated, otherwise for path dependent problems the quadratic convergence is lost.

As a numerical example, bending of a three-dimensional simply supported beam with enforced vertical displacement $w = 0.1$ cm was investigated, see Fig. 4. Supports of the beam were modeled in a way of preventing displacements in all three directions on one side and released displacement in x direction on the other side. The dimensions of a beam were 10 x 2.5 x 2.5 cm with macro mesh division 16 x 4 x 4. At macro level finite elements

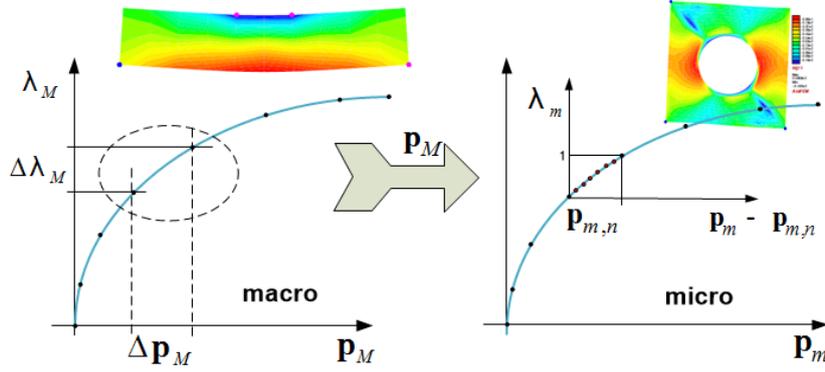


Figure 3: Two-level path following procedure.

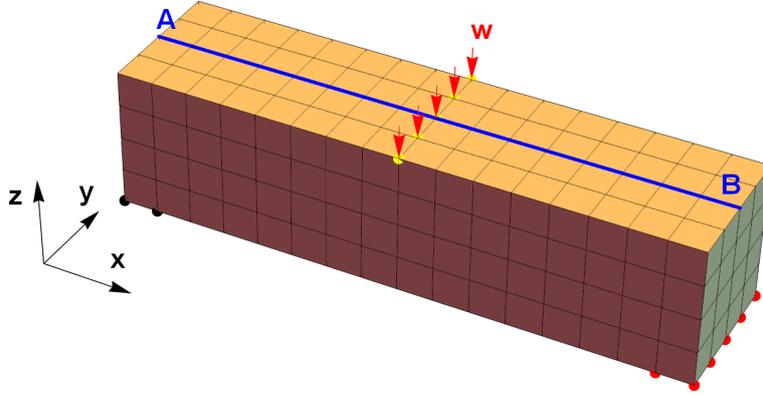


Figure 4: Numerical example: simply supported beam

were hexahedron (H1) and for micro mesh tetrahedron elements (O1) were used. The complete response was evaluated using adaptive path following procedure. The material properties were: Youngs modulus $E = 210$ GPa, Poissons ratio $\nu = 0.3$ and yield stress $\sigma_y = 0.024$ GPa.

Numerical example was evaluated with FE^2 procedure. Results of convergence rate of the Newton-Raphson method for one macro load step in nonlinear region are shown in Table 1, for small strain plasticity (PL). With meaning of labels in Table 1 as follows: PL 1/1 Schur - elasto-plastic material, each macro load step is followed by one micro load step, Schur complement based implementation; PL 1/1 Sens. - elasto-plastic material, each macro load step is followed by one micro load step, sensitivity analysis based implementation; PL 1/5 Schur - elasto-plastic material, each micro increment is divided into 5 substeps, Schur complement based implementation; PL 1/5 Sens. - elasto-plastic material, each micro increment is divided into 5 substeps, sensitivity analysis based implementation, sensitivity is updated; PL 1/5 Sens. uncon. - elasto-plastic material, each micro increment is divided into 5 substeps, sensitivity analysis based implementation, sensitivity is not updated.

In case of sensitivity analysis based implementation of FE^2 convergence is quadratic, while for Schur complement implementation that is not true. Additionally 5 substeps for each macro load step were enforced. In the last column results are shown for case where sensitivity was not updated after every substep, leading to disappearance of quadratic convergence. For MIEL we arrived to similar conclusions as for FE^2 .

Table 1: Comparison of convergence rate for FE^2 scheme

it.	PL 1/1 Schur	PL 1/1 Sens.	PL 1/5 Schur	PL 1/5 Sens.	PL 1/5 Sens. uncons.
1	6.995×10^{-3}	5.004×10^{-3}	5.906×10^{-3}	4.967×10^{-3}	4.974×10^{-3}
2	1.740×10^{-3}	1.186×10^{-4}	9.571×10^{-4}	1.019×10^{-4}	9.569×10^{-5}
3	9.599×10^{-4}	2.888×10^{-6}	7.029×10^{-4}	3.343×10^{-6}	2.566×10^{-5}
4	1.342×10^{-4}	5.568×10^{-9}	4.463×10^{-4}	4.518×10^{-9}	1.846×10^{-5}
5	2.816×10^{-4}		1.404×10^{-4}		1.065×10^{-6}
-	-		-		-
17	1.614×10^{-7}		7.292×10^{-8}		5.825×10^{-9}
-	-		-		
20	1.155×10^{-8}		9.050×10^{-9}		
-	-				
22	5.249×10^{-9}				

Additionally, proposed approach enables unification and automation of various multi-scale approaches for an arbitrary nonlinear, time dependent coupled problem (e.g. general finite strain plasticity). Different multiscale methods FE^2 , MIEL and also single-scale schemes can be used together in one model. With that optimal domain discretization is possible. Implementation of the presented multiscale computational approach in Ace-FEM is fully parallelized for multi-core processors. The setup is also appropriate for the implementation on clusters.

5 CONCLUSIONS

Essential boundary condition sensitivity analysis based implementation of multiscale FE^2 and MIEL was proposed, as an alternative to more traditional implementation based on Schur complement, which is numerically demanding mathematical operation that additionally requires a lot of disc space. The differences between the sensitivity analysis based implementation of FE^2 and MIEL method are in essential boundary condition of micro problem and in essential boundary condition velocity fields needed for the sensitivity

analysis. For FE^2 first order sensitivity is enough, whereas for MIEL second order sensitivity is needed. Ergo, beforehand implementing multiscale methods, efficient analytical sensitivity analysis for first and second order was needed.

Investigation of convergence rate was done on numerical examples for FE^2 and MIEL method, with both ways of implementing them. As a fact, for hyperelastic material, convergence rate is quadratic also for inconsistent sensitivity analysis, regardless of the number of micro substeps, because the problem is not path dependent. The most important asset of automatic-differentiation-based (ADB) formulation and sensitivity based implementation is that quadratic convergence is retained also for nonlinear path dependent problems with substepping at micro level. For path dependent problems only correctly done sensitivity analysis at micro level leads to algorithmically consistent macro tangent matrix and to quadratic convergence. For every substep at micro level, sensitivity has to be updated, otherwise for path dependent problems the quadratic convergence is lost.

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Analysis of a Railway Wheel-rail Connection during Intensive Braking Using Coupled Thermal and Stress FE Simulations

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ABSTRACT

In a railway wheel-rail connection, we can define several tread surface failures of the wheels. This research is focusing on the so-called micro-thermal and sub-surface fatigue cracks. These are two of the most frequent failure types both of the wheel and the rail. The aim of our investigation was to map the appearance and the generation background of these failures using a multistage FE modelling procedure which consisted of coupled transient thermal and elastic-plastic contact FE simulations [1]. During intensive wheel-braking of the railway vehicles, equipped with disk brake only, it appears that the wheel slides on the rail. While the macroscopic sliding speed is restricted it is not eliminated by the WSP (Wheel Slide Protection System). Through the sliding process considerable heat is generated between the connecting parts. This heat may cause micro-cracks on and under the wheel tread. Previously, as it was presented in [2], [3], a modelling method was developed in ANSYS Workbench V14.5 software which could help understand the generation procedure of these micro-cracks caused by the heat generation. In the current state of the research, using an extended FE model, the effect of the different operation conditions (movement speed, different coefficient of friction, etc.) and the coupled effect of the micro-cracks and the subsurface fatigue cracks can be observed. The results showed that which are the sliding speed limits of the WSP systems (beside different braking conditions), where it may not cause micro-cracks on the surface of the wheel tread. Using the results of the elaborated calculations the setup of the WSP systems can be modified under different braking conditions which helps minimize the failures of the wheels and the rail. The recent study and publication was realized within the Knorr-Bremse Scholarship Program supported by the Knorr-Bremse Rail Systems Budapest. [1] P. T. Zwierczyk, "Thermal and stress analysis of a railway wheel rail rolling sliding contact," in Ph.D. thesis, Budapest University of Technology and Economics, 2015. [2] P. T. Zwierczyk and K. Váradi, "Thermal and stress analyses of a railway wheel-rail connection during intensive sliding-rolling braking," presented at the 12th World Congress on Computational Mechanics (WCCM XII), Seoul, South Korea, 2016, p. 1. [3] P. T. Zwierczyk and K. Váradi, "Thermal Stress Analysis of a Railway Wheel in Sliding-Rolling Motion," J. Tribol., vol. 136, no. 3, pp. 031401-1 – 031401-8, May 2014.

TYPICAL AEROSPACE MOUNT DESIGN BY TOPOLOGY OPTIMIZATION AND MANUFACTURED BY ADDITIVE MANUFACTURING

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Key words: Topology optimization; Thermo-elastic; additive manufacturing; SLM; Aerospace bracket

Abstract. Combination of optimization and additive manufacture could make structure optimization, especially for topology optimization, more effectively in improving structure performance and mass reduction. A large load bearing aerospace bracket structure had been design under the guidance of thermo-elastic topology optimization theory and manufactured with additive manufacture method. And on the basic of topology optimization, taking the lightweight structure and optimal performance as ultimate target, taking the necessary installation space requirement into account, the parameterized bracket model had been reconstructed for size optimization. Further, the optimized bracket lightweight structure design had finished. Then, the formability improvement had been done, additional test bars are added in the manufacturing process for performance testing, and process support is added inside the specimen to meet the requirements of the hanging angle process. Finally the bracket was printed with the selective laser melting (SLM) equipment from Bright Laser Technology Company. The mechanical properties test of the test rod shows that the mechanical properties of the specimen meet the requirements. The main contributions are focused on the following points. In order to meet the requirement of thermal load optimization for the aerospace bracket, a new thermo-elastic topology optimization and sensitive analysis formulation had been adopted. The additive manufacture method had been considered in the same processing with topology initial structure reconstruct after topology optimization, which could improve the lightweight level of optimized structure, without the constrain of traditional manufacture requirement, such as openness requirement. In order to cooperate with the SLM equipment, elaborately designed structure rotation and process support had been done, which guaranteed the final structural quality by additive manufacture.

1 INTRODUCTION

Additive manufacturing, which is a technique of layer-by-layer build-up of a product from a computer aided design model^[1], has seen unprecedented growth as a manufacturing tool in some

corporations for reducing mass and shortening reaction cycle^[2]. Additive manufacturing has been adopted in engineering applications^[3-6].

Topology optimization, which is a technique to seek the best structural configuration, has been widely accepted and adopted as an innovative design method^[7] and applications in aircraft, aerospace and mechanical engineering^[8].

Combination of topology optimization and additive manufacturing technologies provides an effective approach for the development of high performance structures. For example, EADS Innovation Works obtained the innovative design of the hinge bracket of Airbus A320 using topology optimization and additive manufacturing technologies. Compared to the original design, a significant mass reduction of 64% is obtained.

Thermo-elastic topology optimization is also extended to the design of compliant mechanism^[9], simultaneous optimization of the microstructure of homogeneous porous material and macrostructure topology^[10] and dynamic compliance minimization in a temperature field^[11]. Besides, multiple materials were taken into account by introducing the concept of thermal stress coefficient (TSC)^[12].

This work focuses on the application of the thermo-elastic topology optimization. An aerospace bracket is designed by thermo-elastic topology optimization and manufactured by additive manufacturing technology. The rest of this paper is organized as follows. In Section 2, the topology optimization method of thermo-elastic structures is introduced. In Section 3, the considered aerospace bracket is presented. In the last section, the conclusions are presented.

2 THERMO-ELASTIC TOPOLOGY OPTIMIZATION

For a typical structural domain Ω , the equation that is solved for the thermo-elastic static linear analysis can be stated as:

$$\mathbf{K}\mathbf{u} = \mathbf{F}^a + \mathbf{F}^{th} \quad (1)$$

Herein, \mathbf{K} is the global stiffness matrix and \mathbf{u} is the nodal displacement vector. \mathbf{F}^a and \mathbf{F}^{th} are the nodal vector of the applied force and of the thermal stress load, respectively. At the finite element level, the element stiffness matrix and the nodal vector of thermal stress load of element e can be expressed as:

$$\begin{aligned} \mathbf{K}_e &= \int_{V_e} \mathbf{B}_e^T \mathbf{D}_e \mathbf{B}_e dV \\ \mathbf{F}_e^{th} &= \beta_e \bar{\mathbf{F}}_e^{th} \quad \bar{\mathbf{F}}_e^{th} = \int_{\Omega_e} \mathbf{B}_e^T \phi \Delta t_e d\Omega \end{aligned} \quad (2)$$

Here, the element strain-displacement matrix \mathbf{B}_e consists of derivatives of element shape functions Δt_e denotes the temperature rise of element e and $\phi = [1 \ 1 \ 1 \ 0 \ 0 \ 0]$ for 3D problems. \mathbf{D} is the elasticity matrix depending on Young's modulus and Poisson's ratio. The thermal stress coefficient β , which can be treated as a material property, is defined as a function of the Young's modulus (E), thermal expansion coefficient (α) and Poisson's ratio (μ)^[12].

$$\beta_e = \frac{E_e \alpha_e}{1 - 2\mu_e} \quad (3)$$

In this work, a minimization of the global compliance subjected to the volume constraint is implemented to obtain the optimal configuration. The formulation of this optimization problem is expressed as:

$$\begin{aligned}
&\text{find: } \mathbf{x} = \{x_i\} \quad (i = 1, \dots, n) \\
&\text{minimize: } C = \mathbf{u}^T \mathbf{K}(\mathbf{x}) \mathbf{u} \\
&\text{subject to: } \mathbf{K}(\mathbf{x}) \mathbf{u} = \mathbf{F}^a + \mathbf{F}^{\text{th}}(\mathbf{x}) \\
&\quad \mathbf{H}(\mathbf{x}) \mathbf{t} = \mathbf{P} \\
&\quad V \leq \overline{vf} \cdot V^{(0)} \\
&\quad 0 < x_{\min} \leq x_i \leq 1
\end{aligned} \tag{4}$$

\mathbf{P} , \mathbf{t} and \mathbf{H} are the global thermal load vector, nodal temperature vector and heat conductivity matrix. Herein, the thermal stress load vector \mathbf{F}^{th} distinctly depends on the design variables while the applied mechanical force \mathbf{F}^a and thermal load \mathbf{P} are assumed to be design-independent.

n is the number of the designable finite elements and subscripts i indicates the i th designable element. \mathbf{x} denotes the set of design variables and a lower bound of the design variables, e.g., $x_{\min}=10^{-9}$ is introduced to avoid the singularity of the structural stiffness matrix and heat conductivity matrix in finite element analysis.

3 TOPOLOGY OPTIMIZATION OF THE BRACKET

3.1 Design processing

In this section, bracket optimization numerical example is tested to illustrate the proposed method. A sensitivity filtering technique is adopted to yield checkerboard-free topology configuration.

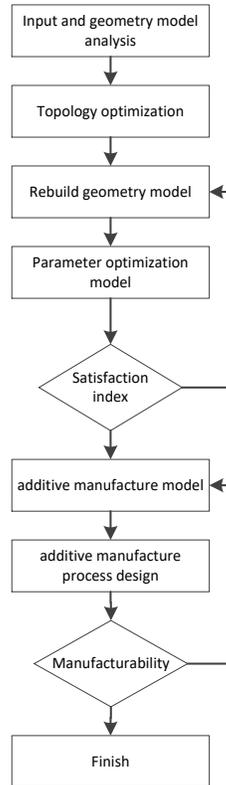


Figure 1 Optimization and additive manufacturing process

The optimization and additive manufacturing flow of the bracket is illustrated in Figure 1, which contains the following steps. First, input and geometry models are analyzed. Based on the initial design structure, the topology optimization space is magnified reasonably, design domain and non-design domain are determined; load and boundary conditions are simplified in this step. Secondly, the topology optimization numerical simulations are carried out to obtain the optimized structure. Thirdly, reconstruct lightweight bracket for additive manufacture based on topology optimization, taking the assemble space, operating space into consideration, the openness requirement of traditional machining is not considered. Fourth, based on the reconstructed geometric model, the parameters optimizations are carried out to complete detail design. Fifth, based on the detailed design model, carry out the process design of additive manufacturing, which including the manufacturing position, auxiliary supporting, et al. Last, finish manufacture of optimized bracket.

3.2 Bracket introduction

A single spacecraft consists of a symmetrical pair of bracket. In theory, the pair of symmetric brackets bear the same load. For assembly process, the asymmetry caused by engine deformation is guaranteed by considering certain safety factor in the bracket design. In this paper, the topology optimization of bracket along the course on the right side is analyzed, and the other side is considered to be completely symmetrical structure. As a centrally loaded component and subjected to certain thermal loads, it is necessary to have good thermal strength and elastic plastic properties, and TC4 titanium alloy material is considered comprehensively.

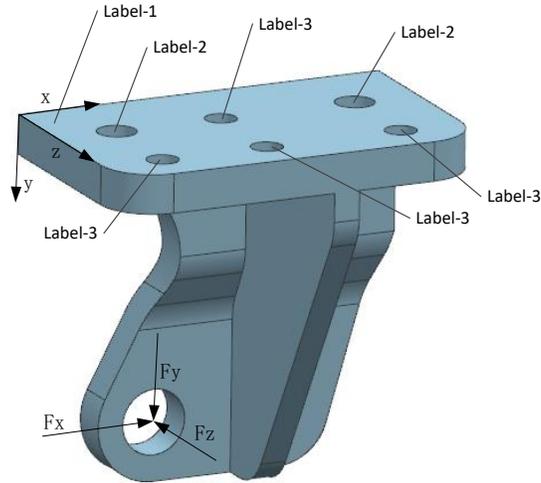


Figure 2 Initial bracket structure and corresponding loads and boundaries

Table 1 Bracket Work Load

Load Direction	X direction	Y direction	Z direction
Load N	-50000	-15000	-7500

Figure 2 display the initial bracket structure, which could meet the functional requirements, but still have potential for mass reduction and stiffness enhancement. The load in bracket includes the following three aspects. Firstly, thrust load of the course direction produced by the engine; Secondly, transverse and vertical mass force load caused by engine self over load; Thirdly, longitudinal frictional force produced by thermal deformation of engine. Consider a certain safety factor, the load in bracket are listed in Table 1.

Table 2 Boundary condition for bracket optimization

Label	Boundary condition	Description
Lable-1	$U_y=0$ $\theta_x = 0; \theta_z = 0$	Bottom face of bracket
Lable-2	$U_x=0, U_y=0, U_z=0$ $\theta_x = 0; \theta_z = 0$	Locating hole
Lable-3	$U_y=0$ $\theta_x = 0; \theta_z = 0$	Bolt hole

The Lable-1 in Figure 2 is the bottom face of bracket. The Lable-2s in Figure 2 are double locating holes. The Label-3s in Figure 2 are four bolt holes. The load and boundary conditions are reasonably simplified, acting on the bottom of the bracket and the connection holes, as shown in Table 2.

The topology optimization was carried out on the basis of re-matching the occupied space of the bracket. Before the topology optimization, the design domain was enlarged so that there would be enough design space in the topology optimization process, the enlarged design space are shown in Figure 3. In addition, according to the previous optimization example, given the necessary non-design domain of the load and constraint boundary, the main transmission line of

the structure can be clearer in topology optimization result. According to the loading and fixing requirements from experiences , give the top margin hole 10mm, bottom hole margin 5mm as the non-design domain, as shown in Figure 3.

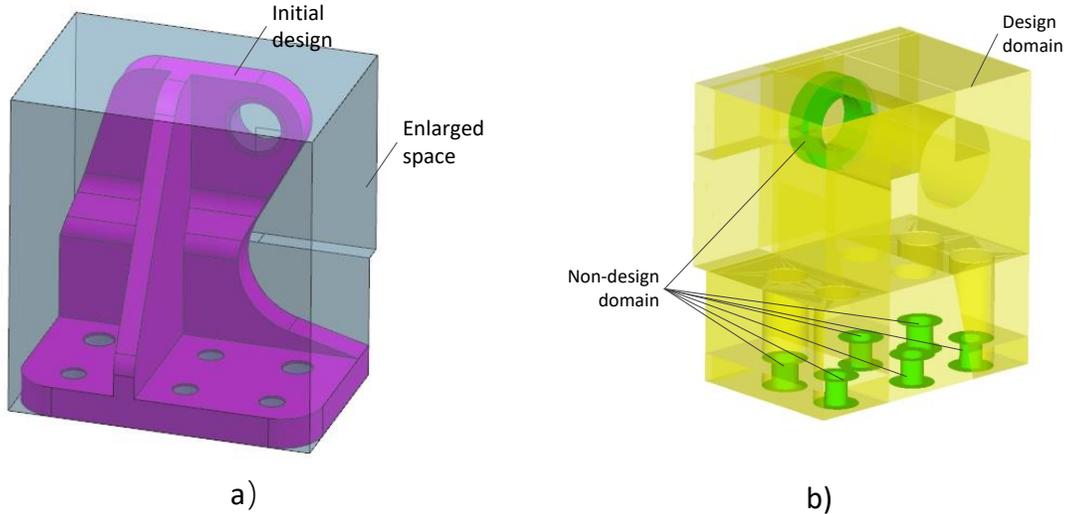


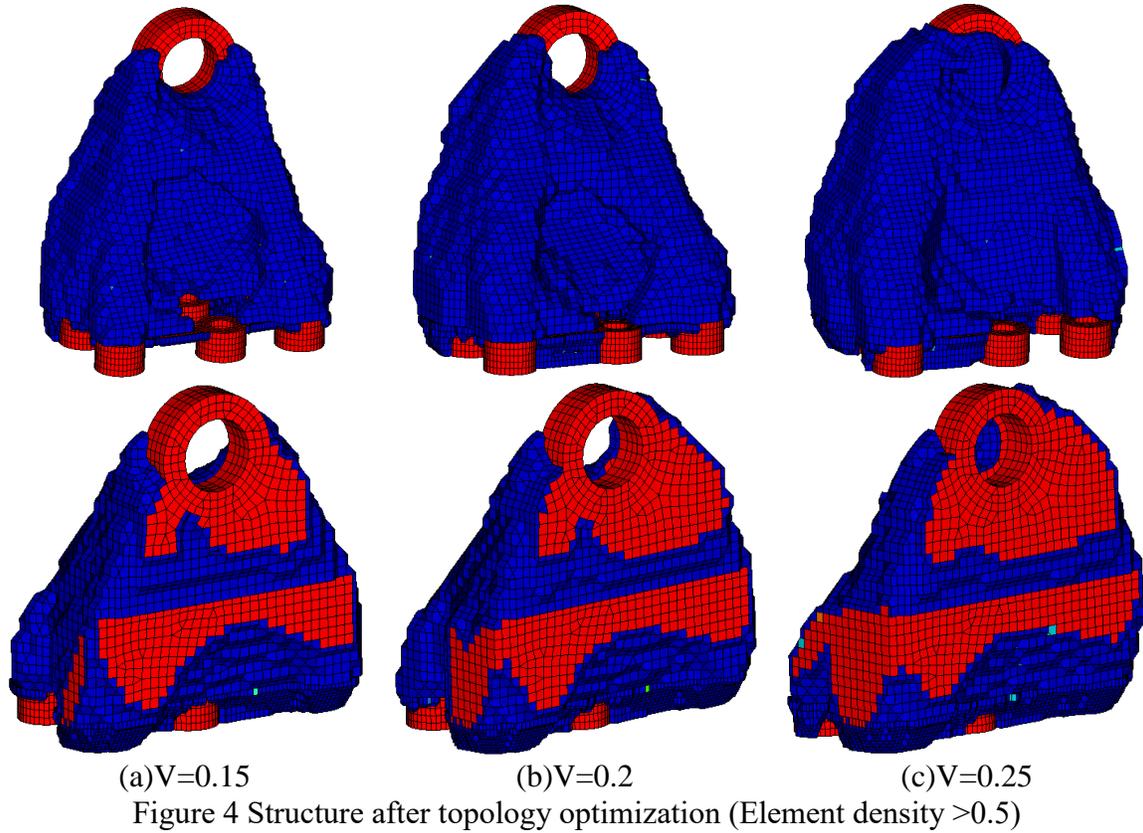
Figure 3 Enlarged space for topology optimization

a) Enlarged design zone; b) Design domain and non-design domain in optimization model

Based on the load, boundary condition and topology model, the optimization formulation is as follows.

$$\begin{aligned}
 & \text{Min: Compliance} \\
 & \text{s.t } \text{volfrac} \leq a \\
 & \text{Dis} \leq b
 \end{aligned}
 \tag{5}$$

Among them, Compliance is the optimized model strain energy, which is the objective function in the optimization process; the optimization constraint contains three kinds of constraints, volfrac is volume fraction constraint, and its upper bound are a, which contains three numbers, corresponding to three optimization examples, the values are as follows: 0.15、 0.2、 0.25. For example, number 0.15 means that the optimized volume does not exceed 15% of the model volume before optimization. Dis is the displacement constrain in load center, and its upper bound is b=0.5mm, which is determined by analyzing the initial bracket structure.



As shown in Figure 4, the optimization results are given under the given volume constraints of 15%, 20% and 25% respectively. The figure gives the optimized material density distribution, which is the density greater than 0.5, the red area is density closed to 1, the density in the optimization result means the corresponding carrying capacity. The numerical examples shows that the volfrac constrain with upper bound 0.15 and 0.2 have better density distribution. The optimized result shown that the material density, distributed between load area and fixed boundary, is closed to 1. The rest of the area forms an approximately boxed structure, which connected the fixed plate and loading hole area at one end.

The model geometry model is reconstructed based on topology optimization results. The following principles are followed in the process of model reconstruction. Firstly, take the function requirement constrain, for example, the bolt installation and operation space. Secondly, refer to topology optimization results as far as possible. Thirdly, in addition to the location of the installation hole, it is not necessary to consider the openness requirements of machining manufacturing, and the manufacturing process limit is considered based on the additive manufacturing method. Fourth, reduce the structural mass as much as possible. Fifth, The stiffness index is not lower than the initial design model.

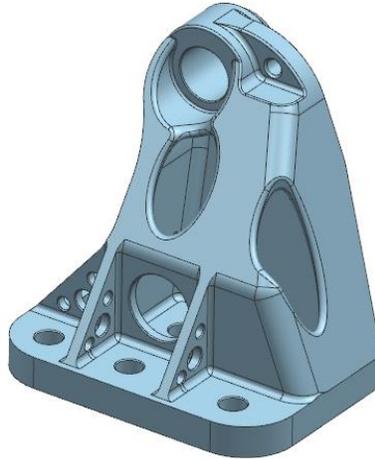


Figure 5 Reconstructed aerospace bracket

Table 3 Comparison of the original and optimized designs

	Mass (kg)	Displacement of KP (mm)	Max von-Mises stress (MPa)	Buckling factor
Existing design	3.48	0.39	400.0	46.7
Reconstructed design	2.85	0.36	635.8	62.0

Comparisons of the original and reconstructed designs are illustrated in Table 2. Benefiting from topology and size optimization, the mass of the aerospace bracket is reduced by 18.1%.

4 Conclusions

A heavy-loaded aerospace bracket is optimized using topology optimization for mass reduction. To meet the requirement of the aerospace bracket design, a formulation of thermo-elastic topology optimization is proposed and the sensitivity analysis is detailed. By means of the adoption of the structural optimization method, more than 18% of the structural mass of the aerospace bracket is reduced and all mechanical performances are satisfied. Following, size optimization based on reconstructed design and additive manufacture by SLM technique will be done.

This work indicates that the combination of topology optimization and additive manufacturing technology provides a powerful tool kit to the engineering designers and they are an amazingly good fit.

Acknowledgements

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Correct Energy Behavior of Stabilized Formulations

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ABSTRACT

Energy errors in the numerical formulation of PDEs can lead to inaccurate results. This occurs in the context of two-fluid flow problems, where many numerical methods create artificial energy at the interface. Even a small energy error can cause highly unstable behavior [1]. This talk concerns the construction of stabilized finite element methods with correct energy behavior. The streamline upwind Petrov-Galerkin method (SUPG), the Galerkin/least-squares method (GLS), and the variational multiscale method (VMS) are very popular stabilized methods of the last decades. These methods are well-established but do not show correct energy behavior. Taking a multiscale point of view, we rectify this discrepancy with dynamic and orthogonal small-scales. The newly constructed methodology is presented for the convection-diffusion equations [2] and the incompressible Navier-Stokes equations [3]. The convection-diffusion case demands the large- and small-scales to be H_0^1 -orthogonal to arrive at a method with desired energy behavior. Its counterpart in case of the incompressible Navier-Stokes equations is to apply an orthogonality induced by the Stokes equations. This needs to be augmented with divergence-free H_0^1 -small-scales to ensure correct energy evolution. The resulting formulation is of GLS-type and enjoys several favorable properties. These include (i) divergence-free solutions, (ii) the conservation of linear and angular momentum and (iii) divergence-free small-scales. A key observation is that the demand for correct energy behavior creates a link between the VMS, SUPG and GLS methodologies. Numerical results show that the dissipation due to the small-scales can be negative in standard stabilized methods. Computations of a turbulent flow show improved energy behavior of the constructed method compared to the standard VMS method. The implementations use the IGA concept (i) to ensure pointwise divergence-free solutions and (ii) to deal with smooth basis functions convenient for the computation of second derivatives. [1] I. Akkerman, Y. Bazilevs, D.J. Benson, C.E. Kees, M.W. Farthing, Free-surface flow and fluid-object interaction modeling with emphasis on ship hydrodynamics, *J. Appl. Mech.* 79: 010905, 2012. [2] M.F.P. ten Eikelder, I. Akkerman, Correct energy evolution of stabilized formulations: The relation between the variational multiscale approach and the Galerkin/least-squares method via dynamic orthogonal small-scales and isogeometric analysis. I: The convective-diffusive context, *Comput. Methods Appl. Mech. Engrg.* 331: 259-280, 2018. [3] M.F.P. ten Eikelder, I. Akkerman, Correct energy evolution of stabilized formulations: The relation between the variational multiscale approach and the Galerkin/least-squares method via dynamic orthogonal small-scales and isogeometric analysis. II: The incompressible Navier-Stokes equations, under review.

The Computational Analysis of Resonances of Bubble Clouds and Fish Schools with the Boundary Element Method

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ABSTRACT

At specific frequencies, schools of fish can exhibit a high reflectivity of acoustic signals from sonar systems, resulting in a strong impact on the quality of the sonar signal used for underwater surveillance. This phenomenon happens for fish that have swim bladders filled with air. Because of the high contrast in density between air and water, a clear low-frequency resonance is present. These resonances, also known as Minnaert resonances, have been observed in practice and can be explained theoretically. Although the resonance frequency of a single air bubble in water can be determined analytically with Mie series, numerical methods need to be used to investigate the impact of the shape as well as the number of bubbles in the system. Specifically, the resonance frequency of a cloud of bubbles depends on the configuration and distances between them. When bubbles are close to each other, high-accuracy numerical methods need to be used to compute the resonance frequency of the coupled system. The boundary element method (BEM) for the multiple traces formulation (MTF) of the Helmholtz transmission problem will be used to analyse the low-frequency resonances accurately. The numerical results are compared with a method based on transmission matrices, demonstrating that the BEM effectively predicts the pronounced frequency shifts in the resonances of the clouds of bubbles. [1] R. Hiptmair and C. Jerez-Hanckes, "Multiple traces boundary integral formulation for Helmholtz transmission problems." *Adv. Comput. Math.*, vol. 37 (2012), pp. 39-91. [2] M. Raveau and C. Feuillade, "Resonance scattering by fish schools: A comparison of two models." *J. Acoust. Soc. Am.*, vol. 139 (2016), pp. 163-175. [3] W. Smigaj, T. Betcke, S. Arridge, J. Phillips, and M. Schweiger, "Solving Boundary Integral Problems with BEM++." *ACM Trans. Math. Softw.*, vol. 41 (2016), pp. 6:1-6:40.

An Adaptive IGA Method for Elasto-capillary FSI

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ABSTRACT

Binary fluids are fluids that comprise two constituents, viz. two phases of the same fluid (gas or liquid) or two distinct species (e.g. water and air). A distinctive feature of binary-fluids is the presence of a fluid–fluid interface that separates the two components. This interface generally carries surface energy and accordingly it introduces capillary forces. The interaction of a binary-fluid with a deformable solid engenders a variety of intricate physical phenomena, collectively referred to as elasto-capillarity. The solid–fluid interface also carries surface energy and, generally, this surface energy is distinct for the two components of the binary fluid. Consequently, the binary-fluid–solid problem will exhibit wetting behavior. Elasto-capillarity underlies miscellaneous complex physical phenomena such as durotaxis, i.e. seemingly spontaneous migration of liquid droplets on solid substrates with an elasticity gradient; capillary origami, i.e. large-scale solid deformations by capillary forces. Binary-fluid–solid interaction is moreover of fundamental technological relevance in a wide variety of high-tech industrial applications, such as inkjet printing and additive manufacturing. In this presentation, we consider a computational model for elasto-capillary fluid-solid interaction based on a diffuse-interface model for the binary fluid and a hyperelastic-material model for the solid. The diffuse-interface binary-fluid model is furnished by quasi incompressible Navier–Stokes–Cahn–Hilliard equations with a preferential-wetting boundary conditions at the fluid-solid interface. To resolve the scale difference between the characteristic length scale of the problem (e.g. droplet radius) and the width of the diffuse fluid-fluid interface we apply an adaptive hierarchical B-spline approximation. we consider a monolithic approach to ensure robustness of the solution procedure for the coupled FSI problem. We consider several aspects of the model, of the formulation and of the considered numerical techniques.

Demonstration of a Computationally Efficient Method for Stacking Sequence Blending of Composite Laminates

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ABSTRACT

Stacking sequence optimisation can be used to increase the strength or stiffness of a composite laminate, or to reduce its weight subject to a strength or stiffness constraint. Optimisation of larger composite structures consisting of multiple panels may result in stacking sequences of adjacent panels that are incompatible with one another. The act of enforcing stacking sequence continuity to ensure structural integrity and manufacturability of a laminated composite laminate is known as blending. This term was first introduced by Zabinsky (1994). In literature, many methods can be found to implement structural continuity by means of stacking sequence blending in one way or another. The complexity of the problem makes the blending of a structure with a large number of adjacent design regions, and thus stacking sequences, prohibitive. This work introduces a computationally efficient method for stacking sequence blending of composite laminates. The presented method is inspired by cellular automata (CA) and relies on the application of a set of simple rules to solve the blending problem. The presented method is demonstrated using the benchmark 18-panel horseshoe blending problem, Soremekun et al. (2002). Each panel is initialized using a genetic algorithm (GA). The result is fed into the CA-scheme. The obtained results are equal to or better than those reported in the literature and were obtained requiring very little operations. This can be attributed to the increased design space of the presented method compared to literature. The computational efficiency makes the presented method especially interesting for composite structures with a large number of design regions. An outlook on the scalability of the presented method and its limits will be given. Soremekun, G. A., Gürdal, Z., Kassapoglou, C. and Toni, D. (2002), 'Stacking sequence blending of multiple composite laminates using genetic algorithm', *Composite Structures* 56(1), 53–62. Zabinsky, Z. B. (1994), 'Global optimization for composite structural design', Monthly technical progress report, under contracts NAS1-18889 (report No. 58) and NAS1-20013, task 2 (report 4).

Interaction Between a Moving Oscillator and an Infinite Beam on Elastic Foundation with Transition Zone in Stiffness – Green’s Function Approach

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ABSTRACT

Transition zones in railway lines are areas between different track structures such as the transition from conventional track (ballasted track) to slab track, to a tunnel or a viaduct. The main feature of a transition zone is that it exhibits a dramatic change in structural behaviour to bridge the difference in the adjacent track parts. This change causes high dynamic loads which contribute to quality deterioration of the track. Two main factors influence the magnitude of the interaction forces between trains and track in transition zones. Firstly, the abrupt change in track stiffness. This stiffness is determined by the mechanical features of the entire track structure; the conventional track is a compliant structure, while slab track, tunnels and viaducts are relatively stiff. A train passing a stiffness change induces a variation of track deflection under the moving dead loads and, consequently, also a variation in the wheelset’s vertical momentum leading to higher (dynamic) loads. Secondly, settlements of the backfill and its foundation are typically larger than those of stiff structures, leading to unevenness of the track. This abstract deals with the issue of the dynamic analysis of an infinite Euler-Bernoulli beam on elastic foundation with transition in foundation stiffness, subjected to a moving oscillator. This model is one of the simplest ones for a vehicle passing a transition zone. The equations of motion are solved by means of the time-domain Green’s function method using convolution integrals in terms of the unknown contact force. Considering the track as an aperiodic structure, the Green’s functions (receptances) are calculated in a stationary reference frame (i.e., non-moving sources). Two methods of solution are investigated. The first one is based on the Laplace Transform, where the response consists of a contribution from the initial conditions and one from the moving contact force. By choosing the initial conditions in accordance with the response of a beam with homogenous foundation subjected to a moving load, the free vibrations and waves due to oscillator entrance are suppressed and steady-state behaviour is achieved before the oscillator reaches the transition zone. The second method is based on the Fourier Transform, which automatically ensures this steady-state behaviour. Both methods are exemplified in the paper. The influence of the length of the transition zone and the speed of the moving oscillator on the contact force are analysed; both sub-critical and super-critical speeds are considered.

Reduced-order Modelling and Design Sensitivity Analysis in Topology Optimization of Geometrically Nonlinear Shell Structures

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ABSTRACT

In structural topology optimization a computational bottleneck occurs in the finite element analysis (FEA) of the physics of the problem [1]. If geometric nonlinearity is taken into account in the analysis of the structural behaviour, then the FEA is an expensive incremental solution procedure (Newton-Raphson) [2]. Reduced-order modelling (ROM) concepts have been employed in the analysis of nonlinear structural behaviour to alleviate the computational burden [3]. ROM techniques are computationally efficient because the bottleneck referred to above is proportional to the number of degrees of freedom in the discretized analysis domain. In this work we study ROM concepts in topology optimization of shell structures subjected to out of plane loading. The aforementioned configuration mitigates numerical issues related to the distortion of low-density elements, which permits, in turn, a focussed study on the computational properties of the ROM in the optimization loop. We present, compare and evaluate sensitivity calculation with four different formulations. In all the formulations the ROM is utilised to speed-up the Newton-Raphson procedure in the analysis phase. The ROM basis vectors are made-up of the orthonormalised solution vectors of a set number of load increments. The first formulation entails correction of the equilibrium solution obtained with the ROM, with the FOM, and a standard full-order adjoint sensitivity calculation. The second formulation is a consistent ROM adjoint sensitivity formulation without full-order correction. The third formulation provides approximate sensitivity information by neglecting the terms associated to the basis vectors in the consistent adjoint formulation. The fourth and final formulation entails projection of the reduced-order solution to the full-order solution space (without correction), and the approximate equilibrium solution is used directly in the standard full-order adjoint formulation. The four options are compared with the standard FOM formulation, which serves as benchmark. The numerical experiments confirm the expected efficiency of the ROM, but the results also indicate that both approximate formulations provide a good balance between accuracy and efficiency. [1] N. Aage, E. Andreassen, B.S. Lazarov, and O. Sigmund. Giga-voxel computational morphogenesis for structural design. *Nature*, 550(7674):84-86, 2017 [2] T.E. Bruns and D.A. Tortorelli. Topology optimization of non-linear elastic structures and compliant mechanism. *Computer Methods in Applied Mechanics and Engineering*, 190(26):3443-3459, 2001. [3] A.K. Noor and J.M. Peters. Reduced basis technique for nonlinear analysis of structures. *AIAA Journals*, 18(4):455-456, 1980

Multiscale Conditional Sampling of PDEs with Random Field Inputs

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ABSTRACT

The statistical prediction and design of physical systems described by partial differential equations with uncertain, complex material properties often carries a prohibitive computational cost. This is attributable to a combination of two bottlenecks: i) the steep cost of evaluating sample paths and ii) the complexity of the underlying parameter space. In order to stay within a given computational budget, some form of adaptivity must be employed. In this talk we adaptively vary parametric complexity, by using Gaussian Markov random fields to model the spatially varying input parameters for our PDE. This allows us to exploit readily available local dependency information of the parameter field in conjunction with standard finite element error estimates and local sensitivities to identify spatial regions that contribute statistically to the error in the computed quantity of interest. We illustrate our approach by means of numerical examples.

Efficient Multiscale/Multiphysics Modeling of Hygrothermal Fatigue in Laminated Composites

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ABSTRACT

Accurate lifetime prediction in composite laminates subjected to a combination of fatigue loads and exposure to extreme environmental conditions is a challenging task. Although of crucial importance in design, a comprehensive knowledge of material behavior under these circumstances is still lacking, leading to inefficient designs with wide safety margins. In order to fill this knowledge gap, it is necessary to move away from traditional characterization techniques based on coupon testing and macroscale modeling and focus on the microscopic mechanisms that drive failure and aging. By explicitly modeling fibers, resin and interfaces, phenomena such as plasticization, hydrolysis, oxidation, molecular relaxation, differential swelling and debonding can be accurately captured. In order to obtain macroscopic information relevant for design, concurrent multiscale techniques providing a continuous two-way coupling between scales can be used. A major obstacle in using such multiscale techniques is the high computational effort involved. Concurrent scale coupling implies that for each macroscopic analysis step multiple micromodels are executed, each of which features dense finite element meshes and high-fidelity constitutive models with expensive stress update procedures. Furthermore, fatigue loads and aging mechanisms usually act in two distinct time scales, leading to analyses with a very large number of time steps. It is therefore important to employ techniques to decrease the effort associated to solving the microscopic equilibrium problem while minimizing any resultant loss of accuracy. In this work, a number of reduced-order modeling techniques is used to allow for fast and accurate multiscale/multiphysics analysis of laminated composites. At the macroscale, the stress equilibrium problem is combined with a Fickian diffusion analysis in order to solve for the water concentration field that drives aging. The micromodels consist of linear-elastic fibers, viscoelastic/viscoplastic/damage resin and cohesive interfaces. The resultant two-scale model is used to predict material degradation after a number of immersion/drying cycles combined with cyclic mechanical loads. In order to accelerate micromodel computation, a combination of the Proper Orthogonal Decomposition (POD) and Empirical Cubature Method (ECM) techniques is employed. In order to efficiently recover stresses and material history at all integration points, Gappy Data least-squares reconstruction is used in combination with a k-means clustering algorithm. The gains in execution time brought by the acceleration techniques are assessed and the resultant lifetime predictions are compared with experimental results.

Experimental and Numerical Multi-scale Mechanics of High Toughness Fibrillating Interfaces with Large Elastic Mismatch

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ABSTRACT

A multi-scale experimental and numerical analysis, encompassing a range of analysis techniques, has been employed to unravel the physical origin behind the remarkably high macroscopic work-of-separation of large elastic mismatch fibrillating interfaces, particularly the copper/PDMS system which is often encountered in stretchable electronics, as function of the interface roughness. The experimental investigation, including 0°, 90°, and 180° peel tests, conclusively revealed that the delamination process is a multi-scale problem spanning all length scales. The progressing peel front was imaged in-situ in an Environmental Scanning Electron Microscope (ESEM). Front-view visualization at high magnification revealed that, at the peel front, a fibrillation process occurs, while high-magnification side-view visualization clearly showed that the fibrils initiate at the peaks of the copper roughness profiles. The fibril shape, distribution and location were found to be governed by the copper topography, which was explained by a mechanism of fibril nucleation resulting from a combination of mechanical interlocking at roughness valleys and cavitation at the roughness peaks. Quantification of the PDMS residue on the delaminated copper surface revealed that the delamination propagates primarily by fibril rupture instead of interface decohesion, while quantitative matching of the two crack surface topologies showed that the PDMS material deforms in a fully hyper-elastic manner. With these microscopic observations at hand, a single fibril model was developed, which was calibrated to dedicated PDMS single fibril experiments. The single fibril simulations showed that, contrary to the frequently used exponentially decaying Traction-Separation Law, the fibril exhibits a nonlinear increase in traction with increasing opening displacement up to the point of a sudden loss of traction due to fibril fracture. A discrete multiple fibril model that incorporates this abrupt fibril rupture was employed to analyze the mutual interaction between the fibrils as well as the local transfer of loads to the adjacent bulk rubber. The high work-of-separation values were explained by the unstable dynamic release of stored elastic energy in the PDMS bulk, the spatial discreteness of the fibrils, including the interaction of the fibrils with the adjacent deforming bulk materials, and the highly nonlinear behavior of the PDMS at large strains. The results established an experimentally validated quantitative relation between the peel front height and the macroscopic interface toughness, which was confirmed by independent results from the 180° peel test.

Redundancy Distribution and Adaptive Structures

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ABSTRACT

Already for the design of a passive load bearing system redundancy and thus the degree of static indeterminacy plays an important role. According to Ströbel [1] the distribution of the static indeterminacy in the system (Figure 1) can be described by the redundancy contribution of each element of a truss. The sum of the redundancy contributions of all elements is equal to the degree of indeterminacy of the entire structure. The extension of this notion presented for truss systems by Ströbel to frames and continua or thin-walled structures yields valuable insight into the load bearing of a structure but at the same time it poses some scientific challenges. Also for the integrative design of efficient adaptive structures in civil engineering the redundancy distribution can be applied. The redundancy matrix, containing the redundancy contributions of all elements, is directly related to the space of adaptability. During the design process the eigen vectors of this space can be used to evaluate how good the stress distribution of a system can be adapted without specifying the number or positions of the actuators. The space of adaptability can also be used to find favourable positions for the actuators taking into account the controllability without application of complex and time consuming optimization algorithms. The aim of this work is to get a better insight into the load bearing behaviour of adaptive systems and characterize them. Thereby an integrative design of optimal adaptive structures based on insights to the load bearing behaviour and not on complex optimization algorithms should be enabled. [1] D. Ströbel. Die Anwendung der Ausgleichsrechnung auf elastomechanische Systeme. Doktorarbeit. Institut für Anwendungen der Geodäsie im Bauwesen, Universität Stuttgart. 1995.

Machine Learning Materials Physics: Hierarchical Multiscale Modeling of Porous Battery Materials by Deep Neural Networks

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ABSTRACT

In this work, we study deep neural networks as a paradigm for abstracting the complexity of porous microstructures of battery electrodes. This investigation is part of a larger exploration of the roles of machine learning in materials physics. The porous electrodes are obtained as arbitrarily chosen configurations of spherical active particles in a fluid electrolyte. Porous separators are similar realizations of cylindrical polymer particles surrounded by the electrolyte. Direct numerical simulations (DNS) are performed for the coupled electro-chemo-thermo-mechanics of the charging-discharging cycle of the cell. Our goal is to incorporate this particle scale physics in homogenized models of the electrode and separator. We have previously used simplified response functions that vary with the evolving porosity in these homogenized models (Wang et al. J. Electrochem. Soc. 164, 2017). Our DNS of the particle scale physics generate training data for deep neural network (DNN) representations of the swelling functions, diffusivity and reaction kinetics. For lithium batteries, the concentrations of Li atoms, Li^+ ions, and porous microstructure variables are the input features to the DNNs. This study offers the opportunity to contrast the DNN representations with previous experimental fits of the response functions that were parameterized by the average porosity.

Constitutive Modelling for Fiber Reinforced Thermoplastic Composites

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ABSTRACT

Fiber-reinforced composite materials offer considerable performance advantages over conventional materials and play a crucial role in light-weight applications, especially for current developments in the field of electro mobility, aeronautical industry, automotive industry etc. However, thermoplastic composites exhibit a highly complex deformation behavior. The understanding of their mechanical behavior, particularly the plastic deformation mechanisms presented by the thermoplastic matrix, is of critical importance to the design and the improvement of their mechanical properties. In this contribution, a microstructural representative volume element (RVE), composed by a thermoplastic polyamide matrix and reinforcement fibers, is initially considered to study the deformation response of these materials. The RVE is subjected to a comprehensive set of stress states and the observed deformation mechanisms together with the nonlinear homogenized response of the composite are analyzed in detail. Based on these micromechanical results, a constitutive model is proposed based on crystal plastic approach and numerically implemented into an implicit integration scheme. The material parameters in the proposed constitutive model are calibrated with micromechanical tests. The proposed model then is used to predict the mechanical behavior of structural composites.

Progressive Damage and Rupture in Soft Viscoelastic Media

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ABSTRACT

Soft viscoelastic media has wide applications, such as tissue engineering and drug delivery. To fully exploit the potential of these materials, the understanding on progressive degradation, damage and rupture in such materials is critical. However, the intrinsic viscoelasticity of these materials hinges the understanding. Here we present an idea which can capture the progressive damage and rupture in soft viscoelastic media, by embedding two essential ideas: a). The free energy of elastomers is not entirely entropic in nature—there is also an energetic contribution from the deformation of the bonds in the chains. This energetic part in the free energy is the driving force for progressive damage and fracture. b). In contrast to the instantaneous nature of the energetically controlled elasticity, the conformational or entropic changes in polymeric materials are processes whose rates are sensitive to the local molecular mobility. The viscous-elastic effects in soft viscoelastic media are considered as effective entropy controlled process in soft media. Using this model, we can estimate the rupture stretch of viscoelastic materials from fundamental quantities describing the polymer network and viscosity of the media. We also demonstrate that in linear viscoelastic region, de Gennes's scaling law is recovered from our model.

Theoretical Views on the Yielding Transition in Amorphous Solids

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ABSTRACT

Glassy systems with long-range interactions often present avalanche type-response under slow driving, whose statistics is similar to that of earthquakes. They also present a vanishing density of excitation at low energy or "pseudo gap". I will explain why these facts must come together, and discuss in particular the plasticity of amorphous solids (for example, how does a mayonnaise flow when one slowly pushes it with a spoon). I will argue that the mean-field description of plasticity maps into the problem of Levy Flights near an absorbing boundary, and draw consequences of this analogy.

Study of Coherent Structures of Turbulent Boundary Layer by DNS and Experiment

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ABSTRACT

To study the characteristics of coherent structures of the turbulent boundary layer, the motion single frame and long exposure imaging (MSFLE) method is proposed and an elaborate direct numerical simulation experiment was also conducted. MSFLE method is a Lagrangian measurement method, the speed of the camera is kept the same as the speed of the coherent structure, and the particle trajectory was captured by long exposure. By calculating the trace of the points on a chosen plane of the DNS result, we can obtain the particle trajectory like MSFLE method. Multilayer of vortex structures was observed and the evolution of the vortex packets with time was recorded. The result of the DNS simulation agrees well with the experiment. The size of the vortex of the different layer is almost the same, and no vortex breakdown was observed. The formation of the small-scale vortex is caused by sweeps and ejections of the larger coherent structures rather than the breakdown process.

Numerical Investigation on Dynamic Mechanical Property of Polyurea by Coarse-Grained Molecular-Dynamics Model

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ABSTRACT

The main goal of this work is to establish relationship between the chain structure and dynamic mechanical properties of polyurea. Molecular-level simulations of polyurea are realized by molecular dynamics (MD). The coarse graining (CG) model is developed to bridge the size disparity from nano to meso scales to reduce the computational cost and make the problem realistic to investigate. The dynamic mechanical properties of polyurea are then calculated from the results obtained by MD simulation using the Green-Kubo method, including the storage modulus, loss modulus and loss factor. They are functions related to frequency, which can characterize the abilities of the material to store and dissipate energy under periodic loading with certain frequencies. The CG procedure mainly includes two parts, static structure mapping and dynamic behavior mapping, respectively. In case of static structure mapping, the all-atoms geometric model of polyurea is divided into the appropriate CG geometric model and use IBI method to obtain the potential energy parameters of the model. Because the dynamics of CG-MD simulations are speed up, it is necessary to revise the dynamic behavior by correcting the time scale and modulus of CG-MD simulation results. MD simulation process is realized by LAMMPS software. The CG method speeds up MD simulation at least four orders of magnitude and makes it possible to study the macromolecule relaxation problems under current computational tool. In order to obtain the macroscopic mechanical properties of the material from the meso scale model, the shear relaxation function is calculated by the Green-Kubo method and then the storage modulus, loss modulus and loss factor are obtained. After confirming reliability of the model described above, the structure of molecular chain is changed, that is the length of chain and ratio of soft and hard segments. Then, the analysis is made for their effect on the dynamic mechanical properties of polyurea. The computational solutions display that if the molecular chain is longer, there is the longer shear modulus, the longer relaxation time, the higher storage modulus and loss modulus. Comparing homopolymer with the same chain length, the copolymer has the higher modulus and longer relaxation time. By reducing the ratio of soft and hard segments, it increases the shear modulus, lengthens the relaxation time and greatly increases the storage modulus and loss modulus. Finally, the CG-MD simulation results are compared with the data from DMA experiments and ultrasonic experiments to verify and calibrate the CG-MD model.

Dynamic Load Identification of Three Dimensional Structures Based on LMS Adaptive Delay Inverse System

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ABSTRACT

The problem of load identification has been a popular research topic in the field of ship and aerospace. Unknown loads usually exist in the dynamic system of the ship or the aircraft which may destroy the structure. For the sake of structural safety and structural optimization, the unknown load needs to be accurately identified. The load identification is composed to the frequency domain method and the time domain method. The time domain method has advantages in the nonlinear problem, which is more suitable for practical complex engineering applications. Based on the LMS Adaptive Inverse Delay System Identification Excitation Method, a three-dimensional acceleration response data identification is proposed to identify the periodic load, impact load and random load time history acting on the three-dimensional structure. The dynamic load can cause multi-directional coupling vibration on the three-dimensional elastic body. The three-dimensional elastic structure is established by Virtual.Lab simulation to obtain the time history data of dynamic load and acceleration responses in different directions. In MATLAB, the LMS adaptive algorithm is used to calculate the load Identify and the recognition effect in different directions are ideal. In a complex structure which is closer to the real engineering structure (double floating valve structure with vibration isolator), the recognition effect of multi-directional coupling vibration response of three-dimensional structure caused by dynamic load is verified by experiment, which proves the feasibility of this method.

Response Analysis of Moving Load on Stepped Cantilever Beam

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ABSTRACT

With the development of modern industry, more and more variable cross-section structure are used in machinery manufacturing, military industry, bridge construction and civil engineering. Beams with variable cross-section show excellent mechanical properties, it will get benefit from studies on variable cross-section structure. In previous research, when concerning about the dynamic response of the variable cross-section structure under moving load, the structures are usually simplified to equal section beam structure. However, the accuracy of the simplified cross-section beam will be reduced, which may not meet the production requirements. In this paper, in order to reduce the deviation, the variable section beams are simplified as ladder beams. This paper will take the stepped cantilever beam as an example, based on the vibration theory and the numerical calculation method, the free vibration characteristics and the forced vibration characteristics of the cantilever ladder beam are analyzed. According to the ladder beam vibration equation and boundary conditions, the natural frequency and mode function of each section of the ladder beam are deduced by using the transfer matrix method. In order to simplify the calculation process, on the premise of guaranteeing accuracy, use the modal truncation method to intercepted the first four natural frequencies for analysis, the first four natural frequencies and the corresponding mode functions are obtained. By using the resulting natural frequencies and mode functions ,under the action of the moving load ,each part of the forced vibration response can be solved by using Newmark algorithm and connect each beam by continuity conditions. The numerical calculation process is done in matlab, the time-response curve of the cantilevered ladder beam under moving loads can be obtained. The research method in this paper can be used to calculate the stepped beam with arbitrary segments and arbitrary boundaries. This research has a good engineering application. Using this method can reduce the calculation deviation and provide data support for designing and manufacturing. This abstract is funded by the International Exchange Program of Harbin Engineering University for Innovation-oriented Talents Cultivation

Visualization Research of Key Blocks of Tunnel in Multi Parallel Fracture Cutting

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ABSTRACT

In order to research key blocks in whole block rock cutted by multiple fractures, take a hydraulic tunnel as an example, based on the analysis of geological datas, achieved the statistics of fractures, average spacing, cohesion, according to block theory, found rock structural plane in three-dimensional network simulation, displayed the movable block of the tunnel, and the display of the most critical block in rocks cutting buy multi groups of fractures, reveal the sliding mode and analyzed the safety factor, satisfied the requirement of the three-dimensional display in the engineering.