Advances in Computational Mechanics with Emphasis on Fracture and Multiscale Phenomena
workshop honoring Professor Ted Belytschko's 70th Birthday.

APRIL 18, 2013 - APRIL 20, 2013

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A New Use of the Elastodynamic Reciprocity Theorem

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Abstract

The reciprocity theorem is a fundamental theorem of the Theory of Elasticity (Betti 1872, Rayleigh 1873). The theorem connects the body forces, the surface tractions and the displacements of two elastodynamic states in a domain of an elastic body, by a volume integral and a surface integral. In this talk it is shown that the reciprocity theorem of elastodynamics can be used to solve actual problems. We consider the example of wave motion generated in a half-space by a time-harmonic force. This fundamental problem is known as Lamb's problem (1904). It is shown that the radiated surface waves, which Lamb obtained by a complicated Fourier transform method, can be obtained from a "back of an envelope" calculation using the elastodynamic reciprocity theorem [1].

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Mechanics of confined thin films, solid (graphene) and fluid (lipid bilayers)

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Abstract

Elastic interfaces are often bound to substrates, and delaminate to form out-of-plane deformation features under lateral stress. For instance, graphene exhibits sharp folds as a consequence of the growth process or its transfer between substrates, which in turn strongly influence its electronic properties and are generally perceived as defects. Here, with analytical models and an atomistic-based continuum model [1,2], we systematically study the wrinkle-to-fold transition in supported graphene, and propose design concepts to precisely control the fold patterns, thereby engineering the properties of graphene through strain. Lipid bilayers form most biological containers at the cellular scale, and are highly dynamical interfaces that undergo continual remodeling. They are commonly confined to adjacent subcellular structures or to artificial substrates and particles. Due to their in-plane fluidity, bilayers buckle out-of-plane when laterally strained by forming tubular or spherical protrusions instead. Through experiments, modeling, and simulations [3,4], we characterize the passive response of confined bilayers, exhibiting a rich behavior generally attribute to proteins in cells. Our findings could help engineer new functionalities into drug delivery systems, such as strain- or pressure-responsive bilayer coated particles.

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Scaling of Probability Distributions of Strength and Lifetime of Quasibrittle Structures:

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Abstract

Understanding the probability distribution of structural strength and lifetime is of paramount importance for the reliability-based design of engineering structures. Since the seminal contributions by Fisher and Tippet (1928) and Weibull (1939), the Weibull distribution, which is one of the three extreme value distribution functions, has been successfully applied to the statistics of structural strength and lifetime for perfectly brittle structures, where the underlying assumption is that the structure can be statistically represented by an infinite weakest link model. The Weibull distribution directly yields the classical Weibull size effect on the mean structural strength and lifetime, which has been used to extrapolate the laboratory testing to structures of different sizes and geometries.

Recent efforts have been directed to quasibrittle materials, which are brittle heterogeneous in nature, exemplified by concrete, fiber composites, ceramics, rocks, sea ice, and many more materials at the micro-scale. These materials have been used for the design of many engineering structures such as buildings, bridges, dams, aircraft, ships, medical implants, MEMs, etc. Substantial amount of experimental data have indicated that the cumulative distribution functions (cdf's) of strength and lifetime of quasibrittle structures cannot be fitted by the Weibull distribution. Recent studies (Bažant and Pang 2006, 2007, Bažant et al. 2009, Le et al, 2011, Le and Bažant 2011) have shown that the inapplicability of the Weibull distribution is due to the fact that for quasibrittle structures the material inhomogeneities are not negligible compared to the structure size, which implies that quasibrittle structures must be statistically represented as a finite weakest link model, where each link represents one representative volume element (RVE). In the formulation of the finite weakest link model, the strength cdf of one RVE is derived from atomistic fracture mechanics and a hierarchical multiscale transition model. With the knowledge of fracture kinetics, the lifetime cdf of one RVE under both creep and fatigue loading can then be further obtained. The finite weakest link model predicts an intricate scale effect on the strength and lifetime cdf's, varying from the Gaussian distribution grafted by a power-law tail for small-size structures to the Weibull distribution for large-size structures. The model also leads to a non-Weibullian size effect on the mean structural strength and lifetime, which agrees well with the predictions by other mechanical models such as the cohesive crack model and nonlocal model.

The finite weakest link model has been found to be in good agreement with the experimentally observed strength and lifetime cdf's of structures made of various

quasibrittile materials such as composites or engineering and dental ceramics. Recent histogram testing on the asphalt mixtures at low temperatures demonstrated a clear size effect on the strength cdf, which can be successfully explained by the finite weakest link model and rules out the possibility of the two-parameter and three-parameter Weibull distributions.

Three numerical methods, namely nonlocal boundary layer model, Taylor expansion method, and random RVE placing method, are proposed to efficiently compute the strength and lifetime cdfs of quasibrittle structures. These methods are used to reanalyze the 1959 failure of Malpasset dam, which demonstrates the important role of size effect in the reliability analysis of quasibrittle structures.

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Advances in Isogeometric Structural Mechanics and FSI

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Abstract

Isogeometric Analysis (IGA) [1] created new and exciting opportunities in structural mechanics discretizations that do not exist in standard FEM. Thin structures, such as shells, beams, and cables are natural for modeling and discretization using IGA. IGA application to fluid mechanics and turbulence was also quite successful from the standpoint of per-degree-of-freedom accuracy. However, the key challenges of automated generation of 3D volumetric shapes for fluid mechanics discretization have not yet been adequately met. Fluid—Structure Interaction (FSI) [2] also benefited greatly from the advances in IGA: Better structural mechanics approximations have lead to increased efficiency, accuracy, and robustness of computational FSI procedures. This claim is supported with good results from a variety of FSI computations, ranging from cardiovascular blood flow to offshore wind turbines.

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X-FEM in Isogeometric Analysis for Linear Fracture Mechanics

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Abstract

This presentation summarizes a collaboration with Professor Ted Belytschko[1]. The extended finite element method (X-FEM) has proven to be an accurate, robust method for solving problems in fracture mechanics. X-FEM has typically been used with elements using linear basis functions, although some work has been performed using quadratics. In the current work, the X-FEM formulation is incorporated into isogeometric analysis to obtain solutions with higher order convergence rates for problems in linear fracture mechanics. In comparison to X-FEM with conventional finite elements of equal degree, the NURBS-based isogeometric analysis gives equal asymptotic convergence rates and equal accuracy with fewer degrees of freedom. Results for linear through quartic NURBS basis functions are presented for a multiplicity of one or a multiplicity equal the degree.

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Deformation and Fracture of Heterogeneous Media using Boundary-Conforming Convected Particle Characteristic Functions in the Material Point Method

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Abstract

The material point method (MPM) saves field data at particles that move relative to a temporary background grid. Particle domains are polygons (polyhedra in 3D) that tessellate the body. Until recently, only conventional FEM basis functions (e.g., tent functions in 1-D) have been used on the grid to solve the weak form of the momentum equation in an updated Lagrange formulation. A new method, called convected particle domain interpolation (CPDI) replaces each FEM basis function with the interpolation of that same function to particle corners [1]. This new CPDI basis inherits linear completeness from the source FEM basis while having the advantage of stretching with particles to avoid numerical fracture while also providing more accurate evaluation of the grid's nodal force and mass integrals (see [2] for an animation). The generalized interpolation material point (GIMP) framework [3] identifies variants of MPM to differ only by their (often implicit) adoption of different "particle characteristic functions" in weighted averages appearing the nodal integrals, but the *de facto* use of approximate weight functions is herein validated. By optimizing the integrand to both particle and mesh topology and also by accommodating more accurate descriptions of angled boundaries (essential for mesoscale simulations), CPDI noticeably improves rate of convergence and achieves stable results in problems that otherwise exhibit spurious numerical fracture caused by fractional particles per cell. These improvements are illustrated through rigorous verification testing via the method of manufactured solutions.

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Mechanics of Nano-Confined Polymers

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Abstract

An issue of paramount importance in nanocomposites, MEMS and microchips is the behavior of polymer under confinement – a nanoscale structure implies that all polymer chains are within 10s to 100s of nanometers from an interface. While the local dynamics of thin polymer films have been studied in detail in the past two decades, development of an understanding of local mechanical properties has been hindered by complex in situ geometries and by the proximity of stiff substrates in simple thin film model systems: mechanical measurements are confounded by interaction with the substrate, convoluting polymer and substrate properties. Several new approaches have been developed to determine local, nanometer scale properties of soft materials, specifically applied to polymers. Nanoindentation and AFM experiments coupled with numerical simulations applied to thin polymer films reveal separately the effects of substrate and interphase near attractive and non-attractive interfaces. Results demonstrate that both surfaces significantly affect the mechanical properties of the polymer up to hundreds of nanometers from the interface. Data also sheds light on the roles of confinement and chemistry on mechanical properties. Our results open the doors to new fundamental understanding of interfacial and small-scale behavior in polymers and other soft materials as well as application advances in nanocomposites, microelectronics and biopolymers.

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Identification of physical fields in biological tissues

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Abstract

Recent progresses in microscopy visualization and image processing techniques enhanced with *in vitro* staining by molecular marking, make it possible to access finer scales in biological tissues. Dual experimental and numerical investigations bring the necessary measurements to calibrate theoretical models and advance the knowledge of cells *in situ* micro-environment. We will present applications of such methods to different biological tissues such as bone, skin and muscle.

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Effects of single crystal plastic deformation mechanisms on the dilatational plastic response and void growth of porous polycrystals

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Abstract

A strong difference between the plastic response in tension versus compression is observed at the polycrystal level, if either twinning or non-Schmid type slip are contributors to plastic deformation at the single crystal level. Despite recent progress in modeling the effects of this asymmetry in yielding, its influence on damage evolution remains a challenge.

In this paper, the combined effects of texture and asymmetric single-crystal plastic deformation mechanisms on the response of voided polycrystals are assessed for the first time. Using analytical homogenization, it is shown that for untextured metals deforming solely by slip, there should be a very specific dependence on the signs of the third-invariant and mean stress that induces a more accelerated void growth than predicted by current models. If the single crystal plastic deformation mechanism is twinning both numerical results using a full-field dilatational viscoplastic Fast Fourier (FFT)- based approach and a recent analytical yield criterion reveal unusual features of the dilatational response, namely a lack of symmetry of the yield surface with respect to both the hydrostatic and deviatoric axes.

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Meshfree Method for Shock Modeling

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Abstract

Shock effects play an essential role in many important physical problems. High rate impulsive loading can generate hydrodynamic processes where shocks give rise to state and field variable discontinuities. Accurate shock modeling requires that two critical issues be addressed: 1) correct representation of the essential shock physics, and 2) retainment of the desired higher-order solution accuracy while avoiding oscillatory instability at the jump. The essential shock physics include the Rankine-Hugoniot (R-H) jump condition and the second law of thermodynamics for entropy production. Oscillatory instabilities in the form of Gibbs phenomenon occur at the jump when higher-order methods are used to approximate the discontinuous solution. The conventional artificial viscosity approach can be overly diffusive and involves an arbitrary numerical parameter, while the Godunov scheme is first-order accurate. Higher- order limiting schemes have been used, but they can also reduce accuracy at smooth extrema. In this work a stable (oscillation limiting) and flux conserved formulation under the reproducing kernel particle method framework is developed for shock modeling. The R-H condition is naturally satisfied and correct shock speed is obtained under the appropriate weak form. A Riemann-embedded flux divergence operator, formulated under the framework of stabilized conforming nodal integration, guarantees correct entropy production and flux conservation and thus produces the correct shock propagation, while a Godunov-type flux-corrected velocity limits shock oscillation. The Godunov velocity correction for oscillation limiting is constrained to the shock region using a detection algorithm based on the reproducing kernel spectral decomposition property, so that higher-order accuracy is maintained elsewhere in the domain. The formulation is introduced here for multi-dimensional scalar conservation laws discretized with an arbitrary nodal distribution.

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Computational modeling of projectile penetration into fiber reinforced ultra-high-performance concrete slabs

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Abstract

This presentation focuses on the computational modeling of projectile penetration experiments on CORTUF, a novel ultra high-performance concrete developed by the US Army. Simulations are based on the Lattice Discrete Particle Model (LDPM) [1] that is a three-dimensional model representing concrete at the meso-scale (10^{-2}–10^{-3} m) and able to include the effect of fiber reinforcement. The method has proven effective in simulating accurately several tests including quasi-static tests like uniaxial, biaxial and triaxial compression, torsion, bending, splitting as well as dynamic experiments.

Prior to the simulation of penetration, the LDPM parameters were identified on the basis of four quasi-static tests. A uniaxial unconfined compression test, a triaxial compression 300 MPa test, and a uniaxial strain test were used to identify the compression parameters; while a 3-point bending test was used to determine the tensile fracturing parameters involved in the material behavior. Furthermore, single fiber pull-out experiments were used to characterize the fiber reinforcing effect.

Finally, without further adjustment of parameters, the behavior of CORTUF slabs subject to a fragment simulating penetrator (FSP) was predicted and compared to the experimental results. For comparisons purposes, the numerical investigation included the analysis of CORTUF with and without fiber reinforcement, as well as of a regular strength concrete composite. Numerical predictions showed excellent agreement with the experimental data.

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Multiscale Analysis of Progressive Failure of Composite Structures

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Abstract

The analysis of composite structures spans many scales, from the constituent level of the matrix and reinforcement to structural analysis. The failure of composite materials has been investigated extensively from the physical and phenomenological points of view, on the microscopic and macroscopic scales.

At the constituent level, the matrix impacs critically the behavior of the composite. It displays nonlinear inelastic behavior and must be characterized under multi-axial loading at different strain rates. A general three-dimensional elasto-viscoplastic model has been developed based on a plastic potential function in strain space [1]. The constitutive relations of the matrix can be incorporated in finite element analyses to predict the behavior of a single lamina, including elastic and strength properties. A scheme is proposed to account for the nonuniform fiber distribution in the composite lamina.

A similar macromechanical constitutive model was developed for the lamina. The model is capable in describing the dynamic behavior under multi-axial states of stress including tensile and compressive loading. It has been validated experimentally for various states of biaxiality, tension and compression, and varying strain rates [2].

A new failure theory, the Northwestern theory [3, 4]], has been developed for predicting lamina failure under multi-axial states of stress including strain rate effects. It is expressed in the form of three failure subcriteria in terms of macroscopic lamina stiffness and strength properties determined by finite element analysis and/or measured experimentally. This theory can be further used in a progressive failure analysis of a multi-directional laminate leading to ultimate structural failure.

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On eXtended Finite Element Methods for Crack Closure

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Abstract

The pioneering work of Belytschko and Black [1] introduced a new way to think about representing crack surfaces into finite element discretizations, culminating in the eXtended Finite Element Method (X-FEM) [2]. Both works focused on crack faces that were opening, without regard to the important problem of crack closure. Whether treated as a contact problem or through the use of cohesive models, crack closure represents a challenging problem for the X-FEM. In this presentation, we discuss how naïve implementations of crack closure can quickly lead to unstable discretizations, and present a recent method [3] that remedies the situation.

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Quadratically consistent integration schemes for meshfree Galerkin methods

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Abstract

Developing efficient methods to integrate the Galerkin weak form is still an open topic in meshfree methods. In the past twenty years, the most successful method is the stabilized conforming nodal integration (SCNI) proposed by Chen *et al.* [1]. However, SCNI can only reproduce a constant strain field in each sub-domain used for integration. Thus, it is not adequate for meshfree methods with quadratic bases, whose strain fields are linear. In this paper, two integration methods which can reproduce linear strain field are presented. They, respectively, use 3 and 1 evaluation point in each background triangle element and are named as quadratically consistent 3-point (QC3) and 1-point (QC1) schemes [2-3]. Patch tests and numerical results of benchmark examples are provided to demonstrate the superiority of the proposed QC3 and QC1 against other methods in terms of accuracy, convergence, efficiency and stability.

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Analysis of 3-D Fractures: A Non-Intrusive Approach Using a Two-Scale Generalized/eXtended Finite Element Method

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Abstract

A non-intrusive implementation of the GFEM^{gl} in a closed-source FEM software is presented. The GFEM^{gl} is based on the solution of interdependent global (structural) and local (crack) scale problems. In the approach presented here, an initial global scale problem is solved by a commercial finite element analysis software. Local problems containing 3-D fractures are solved by an *hp*-adaptive G/XFEM software and an enriched global scale problem is solved by a combination of the FEM and G/XFEM softwares. Interactions between solvers are limited to the exchange of load and solution vectors and do not require the introduction of user subroutines into existing FEM software. As a result, the user can benefit from built-in features of available commercial grade FEM software while adding the benefits of *hp*-adaptive G/XFEMs for this class of problems. This algorithm provides a path for the transitioning of state-of-the-art research codes for engineers and researchers in national laboratories and industries. This transitioning is one of the hallmarks of Prof. Belytschko's career.

10 Years of Progress in Nanomechanical Testing

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Abstract

Nanostructures such as carbon-based nanomaterials (carbon nanotubes-CNTs, graphene and carbon nanofibers-CNFs) and nanowires (metallic and semiconducting) are envisioned as critical components in the next generation of advanced materials and electronic devices. CNTs and graphene, with their outstanding mechanical and electrical properties are now being studied as the building blocks of high-performance composite materials and next-generation electronic and nano-electromechanical systems (NEMS). Crystalline nanowires, with enhanced moduli and fracture strengths as well as active properties, such as piezoelectricity and piezoresistivity, are promising components of future post-CMOS electronics, energy harvesting systems, and ultra-high density interconnects.

Due to this potential, need for accurate metrology, to identify their mechanical and electromechanical properties, has emerged as critical towards the optimization of material synthesis approaches and the design of devices that use such nanomaterials as building blocks. In this talk, we will summarize a decade of progress in the field of nanomechanical testing, from early measurements of moduli by resonance and AFM techniques to state-of-the-art MEMS based techniques that allow *in-situ* electron microscopy measurements of nanomechanical properties. Two case-studies, based on *in-situ* TEM experimentation, will be discussed to illustrate progress in the field and current research trends. First, we will present the measurement of CNT [1,2] modulus and fracture strength, which was found, for the first time, to agree well with quantum mechanical predictions. Then, we will discuss the discovery of unique strengthening mechanisms in penta-twinned silver nanowires and how computational predictions and experimental measurements can be coupled to give a complete picture of activated deformation mechanisms [3].

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DYNAMIC IMPLOSION OF SUBMERGED STRUCTURES: Numerical Simulations and Experiments

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Abstract

The implosive collapse of a submerged, gas-filled structure is a transient, high-speed, fluid-structure interaction problem characterized by ultrahigh compressions, shock waves, large structural displacements and deformations, self-contact, and crack propagation. It is a major area of concern in many underwater engineering applications. The development of a computational framework for this problem is a formidable challenge. It requires incorporating in the computations material failure models, capturing the precise effects on the pressure peaks of many factors such as the rate of structural collapse, and accounting for the various interactions between the external fluid, the nonlinear structure, and the internal gas. This paper presents a computational technology for this problem and discusses its underpinning algorithmic aspects. It also describes two model collapse experiments of cylindrical shells in a constant external pressure environment aimed at investigating the physics of the problem and providing validation data. It concludes with a report on the successful validation of the proposed computational technology and perspectives on the simulation of highly nonlinear multi-fluid-structure interaction problems.

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Fatigue Fracture Analysis using XFEM Combined with Fracture Surface Analysis

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Abstract

Analysis of fractured components subjected to fatigue loads requires applying a variety of analysis techniques to determine the conditions that resulted in the fracture and how to prevent future fatigue fractures. A typical analysis of a fatigue fractured component consists of a microscopic evaluation of the fracture surface to determine such characteristics as ratchet marks, beach marks and striations. Striation spacing on a fatigue fracture surface denotes the crack propagation distance in one cycle. Using these fracture features coupled with fracture mechanics analysis allows the engineer to determine the applied stress and estimate the fatigue life. For complex geometries and loads, numerical analysis techniques such as finite element analysis coupled with XFEM provides a robust and efficient method to compute fracture parameters.

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Interfacial crack propagation: enriched schemes & multi-scale challenges

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Abstract

Damage, fracture and crack propagation are research topics that have played a central role throughout the scientific career of professor Ted Belytschko [1]. Among his published papers, 167 contributions have a hit on these topics. In honour of his contributions, we will focus here on numerical and physical aspects in propagating interfacial cracks.

Interfaces are present in many hybrid materials and systems, whereby cohesive zones are most frequently used at the macro scale to capture the interfacial delamination. Emphasis will be put on intrinsic multi-scale conflicts, triggering ongoing and future research. The interplay between fine scale de-adhesion, intrinsic material dissipation and dynamic dissipation are discussed and the implications for coarse-scale interface models are assessed.

A second aspect relates to enriched schemes, as many were developed in the scientific work of professor Belytschko [2]. The particular computational concern here is the use of a macroscopic discretization length that is larger than the size of the interfacial process zone. This triggers numerical instabilities during crack propagation, which call for an enhanced numerical scheme that traces the moving crack tip inside the cohesive zone element. The essential features of this enriched cohesive zone concept will be explained.

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Multi-scale Modeling of Metals and Composites in Spatial and Temporal Domains: Addressing the ICMSE Initiative

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Abstract

The Integrated Computational Materials Science & Engineering or ICMSE initiative entails integration of information across length and time scales for all relevant materials phenomena and enables concurrent analysis of manufacturing, design, and materials. Computational Mechanics of Materials plays an important role in this integration. This talk will discuss two related thrusts in spatial and temporal multi-scale computational modeling of deformation, failure and fatigue of structural materials. The first thrust area is on crystal plasticity finite element modeling of polycrystalline Ti alloys for predicting cyclic deformation leading to fatigue. Image-based crystal plasticity FEM models are developed, incorporating statistically equivalent distribution functions of grain morphology and crystallographic orientations. A grain-based crack nucleation model evolves from considerations of energy needed to open a free surface in a hard grain surrounded by dislocation pileup in neighboring soft grains. A wavelet based multi-time scale methodology (WATMUS) is developed to significantly reduce the computational time in cyclic loading and deformation till crack initiation.

The second thrust area deals with a hierarchical crystal plasticity model for Ni-based superalloys for three different scales. A sub-grain scale crystal plasticity FEM model scale is developed for micromechanical RVE analysis with explicit depiction of morphology. The model implements a size-dependent dislocation density-based crystal plasticity model with a representation of APB shearing of precipitates. The lowest scale model is homogenized as a function of various microstructural parameters and the activation-based homogenized model is used in the grain scale crystal plasticity model. Finally, a polycrystalline microstructure of Ni-based superalloys is modeled using the homogenized CPFE model for single crystal scale analysis.

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Hydraulic Fracture with XFEM

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Abstract

The recent massive increase in shale (natural) gas production has fundamentally changed the energy landscape of North America. US greenhouse gas emissions have suddenly dropped over the past 5 years and now meet Kyoto targets, in large part, because 8% on US coal-fired generation plants have been replaced by clearer (and cheap) natural gas-fired plants [1]. Shale gas is unlocked from very low permeability shale formations by hydraulic fracturing or fracking. Fracking is a process by which fluid is injected into rock formations at high pressures and rates, causing the rock mass to fracture and leading in huge increases in gas production.

We will present a hydraulic fracture simulator based on the eXtended Finite Element Method developed by Belytschko and co-workers [3-5]. The simulator aims to incorporate the relevant physics while still being a practical tool for field engineers. It couples a linearly elastic continuum model of a fractured body with a Newtonian fluid model between the crack surfaces. Leak-off is integrated through Carter leak-off and power law empirical relations. The mathematical formulation under-pinning the simulator will be presented and several examples will be presented to demonstrate its application.

This presentation is dedicated to Dr. Ted Belytschko who mentorship and many contributions to the computational mechanics community have made this work possible.

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Phase Field Simulation of Polycrystalline Dynamics Based on a Dislocations-Introduced Grain Boundary Model

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Abstract

A multi-dimensional phase field model with built-in dislocation dynamics has been developed to simulate nucleation, growth, and deformation of grains in a polycrystalline system. In this model Peierls-Nabbaro's dislocation potential has been engaged to modify the order parameters that govern phase field evolution; grain boundaries are defined as piled-up dislocation-zones that are mathematically expressed as a function of the gradient of Peierls-Nabbaro potential. The corresponding numerical algorithm has been developed and two/three dimensional computational examples of the single specie polycrystalline system will present.

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Extracting Strain Energy Release Rates from Irwin's integral using higher-order functions in XFEM

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Abstract

Strain Energy Release Rates (SERRs) are computed from Irwin's integral [1], using higher-order crack tip functions [2] for the enrichment of the extended finite element method. By this approach, closed-form expressions provide the SERRs directly from the algebraic degrees-of-freedom, avoiding the need for special postprocessing procedures.

Irwin's integral is taken over a crack extension at the crack tip. The limit of vanishing crack extension simplifies the SERR expressions, with explicit appearance of first-order terms only, yet the result is still effected by the use of higher-order terms in the finite element computation.

Several benchmark examples on pure and mixed mode problems are studied, investigating the effects of the order of the enrichment, mesh refinement, and the length of the crack extension. The results indicate that the use of higher-order enrichment functions is essential for the good performance of this approach, with a particularly significant effect on accuracy when a finite crack extension is considered.

Overall, the approach is found to be simple, efficient, and accurate. The optimal choice of integration limits remains an open question and will be studied in future work.

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Modeling of Dissolvable Electronics

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Abstract

Transient electronics is a class of technology that involves components which physically disappear, in whole or in part, at prescribed rates and at programmed times [1]. Enabled devices include medical monitors that fully resorb when implanted into the human body ("bio-resorbable") to avoid long-term adverse effects, or environmental monitors that dissolve when exposed to water ("eco-resorbable") to eliminate the need for collection and recovery. Analytical models for dissolution of the constituent materials represent important design tools for transient electronic systems that are configured to disappear in water or biofluids [2]. Here, we present solutions for reactive-diffusion in single- and double-layered structures, in which the remaining thicknesses and electrical resistances are obtained analytically. The dissolution time and rate are defined in terms of the reaction constants and diffusivities of the materials, the thicknesses of the layer, and other properties of materials and solution. These models agree well with the experiments for single layers of Mg and SiO_2, and double layers of Mg/MgO. The underlying physical constants extracted from analysis fall within a broad range previously reported in other studies; these constants can be extremely sensitive to the morphologies of the materials, temperature, and the PH value, concentration, and properties of the surrounding liquid.

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Parametric solutions controlling the geometry: a step towards fast shape optimization

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Abstract

Decision-making in engineering design implies determining the optimal choice of many parameters (process parameters, material parameters or geometrical parameters). Usual strategies proceed by defining a trial choice of those parameters and then solving the resulting model. Then, an output-oriented appropriate cost function is evaluated and its optimality checked. This defines an iterative process to reach a reasonable optimum. During this process the design parameters are updated by using a suitable optimization procedure, and then the model recomputed with the updated parameters. Thus, for each choice of the design parameters, a direct numerical solution is recomputed, and, consequently, this has a non-negligible impact on the overall computing time. Here, the focus is on shape optimization, see [1] for a topology optimization approach. That is, determining an optimal set of parameters, which define the geometry of the problem.

In fact, the major contribution is to describe an original approach to compute a rich-enough off-line parametric solution, which can be then particularized on-line for any choice of the geometrical parameters. This allows approximating the solution for any geometry without going back to the resolution of the original boundary value problem. This is possible because the parameters are introduced as extra-coordinates. In fact a sort of computational vademecum is evaluated in the off-line stage to allow evaluating the approximation for a given set of geometrical parameters on-line and consequently very rapidly.

Introducing a large number of extra-coordinates implies increasing the dimension of the problem. Nevertheless, assuming the separated representation of the solution and using a Proper Generalized Decomposition (PGD) circumvents the curse of dimensionality, see [2,3]. Here however, this approach is a first attempt to compute solutions with domains whose geometry is parameterized and these parameters are extra-coordinates.

The parametric representation of the geometry relies in a proper mapping, which induces a separated representation in the weak form of the boundary value problem. Considering a set of piecewise-linear mappings has alleviated the inherent difficulties associated to lack of separability for the inverse of the Jacobian of a general transformation.

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The Chicken and Egg Problem of Computational Mechanics

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Dedication

Dedicated to Ted Belytschko, a great friend for 38 years and counting.

Abstract

When the workshop was first being organized, Ted was interested in the speakers addressing certain assigned topics. My assignment was discretization methods. Subsequently, the format of the conference was changed but I had already thought about what I might say about discretization in computational mechanics. My thinking led to some ideas that I would like to describe in this short presentation. The ideas run contrary to what has become accepted in computational mechanics. To make a long story short, the question is: What determines the variational method that you employ? It seems everyone accepts the Galerkin method as given and you just substitute whatever functions you are fond of in it and off you go. However, I think the functions and the variational method to be employed provide a chicken and egg conundrum that can only be solved by crafting one to fit the other. I believe that the finite element method actually went through such soul searching in the late 1950s and early 1960s and I will describe some of the history of that time. This issue is important in the present because many new functions spaces have been recently proposed and so far used almost exclusively in conjunction with the Galerkin method. I will argue that a variational formulation other than Galerkin may be more appropriate in these cases. In addition to the historical arguments, I will provide some performance results to support my conclusions.

Some Contact Problems Showing the Influences of Inhomogeneities

By
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In this talk the general theory of eigenstrains as developed by Mura and others will be applied to show the influence of inhomogeneities on bodies in contact. Solutions, which have been derived for the point eigenstrain and cuboidal inclusion problems, will be utilized to solve contact problems, whose bodies may contain an inhomogeneity. Specific examples that will be outlined are the following: 1) Contact involving two joined quarter spaces, 2) Partial-Slip contact involving an inhomogeneity, and 3) Partial-Slip contact involving plasticity.

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Multi-scale modelling of fracture: a continuous-discontinuous computational homogenization approach

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Abstract

Throughout his career, Prof. Ted Belytschko has contributed extensively into the advancement of the computational methods for fracture, with in the last decade particular emphasis on the incorporation of the multi-scale nature of damage and fracture into numerical techniques [1].

In line with Ted's work and interests we will present a new computational homogenization technique for the multi-scale modeling of materials from microscale damage initiation and development up to the point of macroscopic failure. The proposed continuous-discontinuous computational homogenization-localization framework involves a discontinuity enriched macroscale problem, which can be described within either embedded discontinuities or partition of unity based XFEM [2] concepts. The underlying microstructural volume element (MVE) is crossed by a band with high strains, i.e. the strain localization band. For the multi-scale coupling, special scale transition relations have been established that involve the material response of the bulk and the localization zone, obtained from the same MVE analysis. This constitutes the most important distinguishing feature of the developed approach.

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Finite element elasticity of anisotropic materials with single-quadrature-point hexahedra, selective reduced integration and nodal-integration stabilization

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Abstract

Selective reduced integration (SRI) has been known for a long time to lead to quite useful improvements of element performance in almost incompressible elasticity. The equivalence of SRI with mixed methods promises robustness for certain element configurations. The limitation was so far that the material needed to be assumed isotropic. We use recent results on anisotropic constitutive response splitting to construct a useful FEM for anisotropic elasticity based on SRI in which one-point quadrature hexahedral elements are stabilized with nodal integration.

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Universal Meshes for the Simulation of Hydraulic Fractures

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Abstract

We describe our approach to simulating hydraulic fractures based on the use of Universal Meshes. This problem is challenging to simulate because of the non-linear coupling between the fluid pressure and the crack opening, and also because of the presence of two moving boundaries, the crack tip and the fluid front. Often in simulating hydraulic fracture, the rock is modeled as a homogeneous, isotropic, infinite elastic medium. This has the advantage of bypassing the 2D elastostatics equations for the rock and instead solving a 1D integral relation between the fluid pressure and crack opening. While this approach has been highly successful for this simplified case, there would be great difficulty in extending it to more general problems, for example when it is desired to model the effects of poroelasticity or the intersection of hydraulic fractures with pre-existing natural fractures. Finite-element-based approaches are attractive in the simulation of hydraulic fractures because of their ability to easily handle inhomogeneities in the material and more general geometries.

Constructing finite-element-based approximations for hydraulic fracture problems faces a crucial obstacle though: a suitable mesh is needed over the faces of a possibly-curved-crack to solve for the pressure distribution in the fracturing fluid. Since the crack itself is part of the solution, it is not possible to a priori know where the crack will be and hence where to construct such mesh. Standard solutions for crack propagation, such as cutting elements as in the extended finite element method, lead to very irregular meshes over the crack surfaces not suitable for computation. Such meshes can lead to accuracy and conditioning problems.

To this end, we have introduced the idea of a Universal Mesh. A Universal Mesh is one that can be used to mesh a class of geometries by slightly perturbing some nodes in the mesh, and hence the name universal [1,2,3]. In this way, as the crack evolves, the Universal Mesh is always deformed so as to exactly mesh the crack surface. The advantages of such an approach are: (a) the crack faces are exactly meshed with a

conforming mesh at all times, and the quality of the surface mesh is guaranteed to be good, (b) apart from duplicating degrees of freedom when the crack grows, the connectivity of the mesh and the sparsity of the associated stiffness matrix remains unaltered; this has the positive effect of enabling efficient iteration over the crack geometry, needed for the satisfaction of Griffith's criterion at the crack tip.

We have devised one algorithm to simulate plane-strain, straight [4] and curvilinear hydraulic fractures that takes advantage of a Universal Mesh. The algorithm is capable of handling the non-linear coupling between the pressure and crack opening profile, and to separately track the evolution of the fluid front and the crack tip. For straight fractures, we validate the algorithm by exactly reproducing some asymptotic exact solutions.

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Multiscale Crystal Defect Dynamics: A process zone approach

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Abstract

In this work, we present a novel multiscale crystal defect dynamics (MCDD) that is based on an atomistic-informed multiscale process zone (AMPZ) finite element method. We apply it to simulate dislocation motions and fracture in crystalline solids. The main technical ingredients of the multiscale crystal defect dynamics are: (1) Process zone super lattice model of crystalline solids and defects; (2) Embedded atom method (EAM)-based constitutive modeling of materials and defects; (3) High order Cauchy-Born rule-based strain gradient formulation for different order of process zones, and (4) Barycentric finite element technique for polygonal and polyhedral defect finite elements. The proposed multiscale crystal defect dynamics (MCDD) provides an efficient and viable alternative between atomistic molecular dynamics and elastic dislocation dynamics for simulations of defect evolutions such as voids, dislocations, and grain boundaries, twin boundaries, etc. In particular, MCDD provides a mesoscale description on both dynamic lattice microstructure and defect microstructure, and their interactions. The method may provide a multiscale solution for simulation of nanoscale or mesoscale polycrystalline plasticity.

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Microstructure Model for Carbon Nanotube Reinforced Composites Based on Material Point Method

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Abstract

Carbon nanotube (CNT) reinforced composites have drawn great attention owing to their outstanding mechanical, thermal, and electrical properties[1]. But the numerical simulation has not been well addressed because of the complex microstructure of CNT composites. It is difficult to construct a microstructure model close to the real material based on the conventional finite element method due to curved and disordered tubes and high volume fraction.

In this talk, we present a new falling method to model the microstructure based on material point method (MPM). MPM, as one kind of meshfree particle methods, utilizes a set of Lagrangian particles (called the material points) and a set of Eulerian background mesh. As possessing both the advantages of Lagrangian and Eulerian descriptions, MPM is very appropriate for problems of extremely large deformation[2]. Adding or removing material points is very convenient owing the meshfree property. The treatment of contacts between different bodies is also convenient and efficient.

In our new method, the CNTs are firstly discretized by material points and randomly placed in a box. Then the CNTs fall to the ground under the gravity force to form the skeleton of the microstructure model. The CNTs may contact and interact with each other but no penetration or overlapping exists. Then the matrix particles are inserted into the gaps between the CNTs. A microstructure model of the volume fraction close to the experiment is obtained, and all the CNTs in the model are curved tubes. The macroscopic mechanical properties are investigated based the microstructure model, and the influences of the volume fraction and the properties of CNT connections are studied as well.

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XFEM modeling of ultrasonic wave propagation in polymer matrix particulate/fibrous composites

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Abstract

A method for representing discontinuous material properties in a heterogeneous domain by the extended finite element method (XFEM) has been applied to study ultrasonic wave propagation in polymer matrix particulate/fibrous composites. Representative volume elements of the composite material microstructure were generated by the random sequential adsorption(RSA) algorithm, where level set fields represent the matrix/inclusion interfaces within the domain. The equations of motion were integrated explicitly in time with mass lumping on the nodal and enriched degrees of freedom. This method shows improved agreement of the wave attenuation coefficients(WAC) from experimental measurements of ultrasonic, longitudinal waves in particulate composites compared with analytical methods, especially for the high volume fraction. The WAC were also computed for fiber composites, including random and aligned fiber orientations. Our results suggest that fibers aligned with the direction of wave propagation produce the greatest amount of attenuation, where scattering is the dominant energy attenuation mechanism when the wavelength approaches the characteristic length of the microstructure.

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A Discontinuous/Continuous Galerkin Method for Modeling of Interphase Damage in Fibrous Composite Systems

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Abstract

A Discontinuous Galerkin (DG) interface treatment embedded in a Continuous Galerkin formulation is presented for simulating the progressive debonding of bi-material interfaces. The method seamlessly tracks the progression from perfect adhesion to interface softening and finally to complete separation without resorting to node-to-node springs or deletion of connectivities. Specifically, the combination of damage and friction along the debonding surface is easily accommodated by borrowing concepts from multi-surface plasticity. Another benefit of this framework is a built-in error estimator that provides quantified feedback on the discretization error in the simulation results. We present a simple yet accurate error estimator that is computed during a post-processing step. The study of fibrous composites serves as the application the proposed method. The constitutive behavior of the interface is modeled within an energetic framework from which the initiation criterion and softening response emanate. Numerical simulations are conducted for various loading cases on fiber-matrix unit cells that highlight the performance of the method on crude meshes.

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High performance three-dimensional multiscale modeling of failure in heterogeneous adhesive layers

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Abstract

Modern adhesives have complex microstructures, often containing rubber particles and carbon nanotubes to increase fracture toughness or small metal flakes to increase secondary functionalities of thermal or electrical conductance. Understanding how the inclusion of these particles to the adhesive layer changes the overall structural performance of the bonded system is an important question in engineering application. Simulating a macroscale bonded system with the resolution required to resolve microscale failure effects in the heterogeneous adhesive layer is prohibitively expensive. Thus a multiscale method capable of coupling microscale failure processes to the macroscale response is required. Furthermore, high performance computing is necessary to solve the large system of equations resulting from the fine discretization of the complex geometry and failure zones at the microscale.

Expanding on our earlier work in the 2D small strains setting [1,2], we have formulated a fully coupled, 3D finite strains model with damage mechanics at the microscale. The model is formulated in the spirit of FE^2 computational homogenization, attaching a representative microscale domain to each integration point in the adhesive layer and linking the micro- and macro-scales by the variational energy equivalence. Results of high performance (parallel) 3D multiscale simulations on model adhesive layer microstructures are presented and examined. We will focus on microstructures with varying sizes and volume fractions of embedded spherical particles.

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The Thick Level Set model : an efficient theoretical and numerical localization limiter for strain softening in dynamics

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Abstract

The use of strain softening models in transient dynamics is known to be problematic due to contributions from Belytschko et al. [1-4]. Finite element simulations yield a dissipation highly dependent on the mesh size. The culprit is the local character of the constitutive law which lacks a characteristic length. The source of the problem is in fact not a numerical one but a theoretical one. Indeed, analytical solutions [2] exhibit infinite strain over a set of zero measure.

To remedy this spurious localization issue, rate dependent damage models have been proposed, as delayed damage type models [5]. These models introduce a time-scale and indirectly a length scale when it is multiplied by the wave speed. Regarding implementation, these models are nice since the constitutive law is local. Unfortunately, for very slow loading of fast loading with small energy, these models still exhibit spurious localization. Another class of remedy, is to inject directly a length scale in the model [3,4]. Unfortunately, this requires time consuming operations which are incompatible with a usually fast explicit dynamics solver.

We will detail a new approach coined Thick Level Set [6] coupled to delayed-damage [6]. It combines the introduction of both a time scale and a length scale while preserving an efficient implementation on top of explicit dynamics schemes. Numerical implementation will deal with brittle models in transient dynamics.

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Large deformations near a crack tip in a fiber-reinforced Neo-Hookean sheet

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Abstract

The asymptotic fields at the tip of a crack in a fiber-reinforced Neo-Hookean sheet are derived. The investigation is carried out for the case of a strain energy function for a fiber-reinforced hyperelastic material motivated by composite mechanics Guo et al. [1-3]. The resulting asymptotic deformation and stress fields depend qualitatively and quantitatively on the degree of fiber reinforcement. For suitable choice of parameters, the strain energy potential for the material reduces to that of a pure Neo-Hookean material and the corresponding asymptotic fields to those obtained by Knowles and Sternberg [4]. The result obtained may provide useful crack tip enrichment fields for computational modeling of composite materials including soft biological tissue reinforced by collagen fibers.

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Probability bounds analysis non-linear structures

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Abstract

A probability bound analysis provides solutions to structural analysis as a set of possible continuous cumulative probability distributions CPD) defined by upper and lower bounding function. With such a representation, aleatory uncertainty is represented by a CPD which is an element of the set while epistemic uncertainty is quantified by the width of the bounds. Such sets are known as a probability box or a p-box [1, 2]. In the absence of epistemic uncertainty, p-box formulations reduce to conventional probabilistic analysis. In this paper we will present methods for calculating the non-linear response of structures in terms of p-boxes. The formulation is based on a linear interval Monte Carlo method [3]. A non-linear interval finite element method that provides tight bounds on non-linear structural response to interval loading is critical to the non-linear Monte Carlo p-box. We present methods that provide for these sharp bounds including: various forms of interval extensions to non-linear constitutive modal, mixed methods for sharp stress and strain calculations, and mixed interval/non-interval iterative non-linear equation solvers. We will examine scenarios where external loadings are described in terms of a mix of p-boxes and conventional random variables. Constitutive models include Ramberg-Osgood, and piecewise-linear plasticity models. Example calculations for various structures will be presented and discussed. The behavior of the nonlinear p-box analysis methods will be described.

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Porosity Evolution and the Thickness Debit Effect in Superalloy Single Crystals

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Single crystal Ni-based superalloys were introduced in the early 1980s and since then have been widely used in turbine aerofoils in jet engines. The desire for weight reduction and the use of advanced metal cooling schemes tends to drive designs toward thinner airfoil walls. Creep tests on Ni-based superalloy specimens have shown greater creep strain rates and/or reduced creep rupture times for thinner specimens than is predicted by current theories. This is termed the thickness debit effect. To investigate the mechanism of the thickness debit effect, isothermal, constant nominal stress creep tests were performed on uncoated PWA1484 Ni-based single crystal superalloy sheet specimens with two thicknesses and under two test conditions: 760 deg. C/758MPa and 982 deg. C/248MPa. The specimens contained initial micro-voids formed during the solidification and homogenization processes. The experiments showed that porosity evolution could play a significant role in the thickness debit effect. This motivated basic mechanics studies of porosity evolution in single crystals subject to creep loading. Three-dimensional finite deformation finite element analyses of unit cells containing a single initially spherical void were carried out for various values of stress triaxiality and various values of the Lode parameter. At low values of the stress triaxiality, well separated voids can collapse into crack-like or needle-like shapes. On the other hand, if the voids are sufficiently close the voids can coalesce. Depending on void spacing, there is a transition between void collapse and void coalescence. Implications for the thickness debit effect will be discussed.

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Interaction of a Shock Wave with Elastically Constrained Periodic Obstacles: Estimates and Visualization

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Abstract

We have studied the interaction of shockwaves with periodically distributed, elastically constrained obstacles, using a Schlieren setup in conjunction with two cameras, one a high-speed to visualize the interaction of the shockwave with obstacles, and the other to record the elastic response that results as the shockwave imparts initial velocities to the obstacles. The first event takes place in 10's of microsecond, while the elastic vibration occurs relatively long time afterwards, about fractions of second. First the interaction of shock with a single obstacle is examined, revealing complex pressure distribution behind the obstacle. Then two and more obstacles are considered, showing fascinating shock interactions and elastic behaviors. A simple tabletop shock tube was created for this experiment. It produces controlled, reproducible shockwaves useful for observing the shockwave interaction with the obstacles and the resulting dynamic effects with potential application in shock mitigation.

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Validation of Multiscale Models of Complex Systems

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Abstract

This presentation addresses issues of selection, calibration and validation of multiscale models of complex physical systems. Applications include molecular models of polymeric materials. A Bayesian framework is described that permits the development of rigorous theories for coarse graining of atomistic models, consistency and relative entropy of statistical mechanics formulations of atomistic and molecular models, selection of molecular interaction potentials using the idea of model plausibility, and the use of fine scale information to design validation experiments and estimate model discrepancy. Alternative notions of model validation processes are described and compared.

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ADVANCES IN THE PARTICLE FINITE ELEMENT METHOD (PFEM) FOR PARTICULATE FLOWS IN ENGINEERING

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Abstract

We present recent developments in the Particle Finite Element Method (PFEM, www.cimne.com/pfem) for analysis of complex particulate flow problems in engineering .These type of flows are typical of fluid-soil-structure interaction situations, environmental flows, biological flow, melting and burning of objects in fire and some industrial forming processes, among others [1].

The PFEM uses an updated Lagrangian description to model the motion of nodes (particles) in both the fluid and the solid/structure domains which are modelled as a single continuum (SC). Nodes are viewed as material points which can freely move and even separate from the main analysis domain representing, for instance, the effect of physical particles or water drops . A mesh connects the nodes defining the discretized domain where the governing equations for the SC problem are solved as in the standard FEM. The necessary stabilization for dealing with the incompressibility of the fluid is introduced via the finite calculus (FIC) method. An incremental iterative scheme for the solution of the non linear transient coupled problem in the SC is used. Advances in the PFEM to allow for frictional contact conditions and surface erosion at fluid-solid and solid-solid interfaces via mesh generation are described. A new technique to model the motion of particles of different sizes in a fluid is described.

We present examples of application of the PFEM to a number of particulate flow problems such as the erosion of earth dams in overtopping situations, the motion of mud particles and floating/submerged bodies in tsunami flows, the impact of slurry flows on structures , the erosion due to water streams in river beds and slopes, wall erosion and particle transport in excavation and drilling problems in the construction and oil/gas industries, melting and dripping of polymer objects due to fire and simulation of industrial forming problems involving particulate flows ,among others.

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Multiscale Spatio-Temporal Modeling of Fatigue Failure in Composites

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Abstract

We present a multiscale modeling methodology for failure prediction in composite materials subjected to cyclic loading [1]. The proposed methodology is multiscale in time, to account for the size disparity between loading periods and characteristic times associated with damage accumulation, as well as space, to account for the size disparity between the characteristic lengths of the composite structure and the underlying constituents. The proposed approach is a space-time generalization of the computational homogenization method, where the primary issue of computational complexity is addressed by reduced order modeling in both space [2] and time. We will focus on the discussion of a novel fast multiple time-scale integration strategy that significantly increases the computational efficiency of structural life prediction analysis. In the proposed strategy, the elastic time stepping is employed in solving microchronological (i.e., fast time scale) problems, whereas the inelastic equilibrium is satisfied at each step of the macrochronological (i.e., slow time scale) problem. We demonstrate the efficiency and accuracy characteristics of the proposed approach and discuss preliminary investigation of the damage accumulation behavior of CFRP composites subjected to cyclic loading.

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A quantum mechanics/continuum mechanics method applied to the study of graphene fracture

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Abstract

A new technique has been developed to study fracture in nanomaterials, in which quantum and continuum mechanics are coupled. A key feature of the method is that broken bonds are identified by a sharp drop in the quantum-mechanical electron densities at crack tips. As fracture occurs, the tip positions and crack paths are updated in the continuum mechanics, from the broken bonds in the quantum mechanical (QM) models. As the simulations proceed, the QM models are centered on the crack tips to adaptively follow their courses, making it possible to trace paths with complicated geometries. The method is applied to the study of grapheme fracture, and incorporates a constitutive equation which we have recently developed. The displacement fields necessary to make estimates of quantities such as critical stress intensity factors and crack paths could only have been applied accurately to sheets that are much too large for QM models, while the use of quantum mechanics is essential for the accurate modeling of the propagation of the crack tips.

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Multi-Timescale Approaches to Investigate Plasticity in Amorphous Solids

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Abstract

We utilize the recently developed self-learning potential energy surface metabasin escape algorithm to probe the yield mechanisms of a two-dimensional amorphous solid for temperatures under the glass transition, and for strain rates from atomistic to experimental. We find a generic transition in the yield mechanism that is characterized by a sudden change in the direction of shear localization from parallel to nearly orthogonal to the loading direction at reduced strain rates, elevated temperatures, or a combination of both. The existence of this generic transition demonstrates that unexpected yielding mechanisms may occur if a deformed atomistic system is allowed to explore all possible relaxation pathways.

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A Thermomechanically Implicit Coupled Approach for Damage and Crack Propagation.

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Abstract

Advanced high-strength steels, aluminum or titanium alloys are gaining popularity in automotive and aeronautics applications because they exhibit a large ductility for a high strength level. As a result, these newly developed alloys are ideal for crash energy management, fatigue and durability of sensitive parts. With proper design strategy, these materials offer a great opportunity for weight reduction and crash performance. Therefore, the characterization of the mechanical properties of these materials has to be performed in the context of rate dependent plasticity at large strains and for both low and high strain rates.

In a finite element simulation of high strain rates phenomena, three main ingredients have to be taken into account. At first, adequate constitutive modeling including strain rate and temperature effects must be used to take into account high strain rate and the thermal softening of the material. Secondly, the study of fast phenomena such as crash must include a large strain formulation, as well as inertia effects. Thirdly, numerical solution algorithms have to evaluate accurately the evolution of positions and temperature all along the process.

Beyond thermomechanical constitutive equations, a general formulation including material damage, possibly coupled with element erosion to simulate crack propagation is proposed. These damage laws are able to describe the loss of strength of materials both for quasi-static phenomena as well as for dynamic problems.

In this lecture, we will present a consistent formulation able to take into account all the mentioned effects, including a fully implicit approach for element erosion due to damage in order to simulate crack propagation. The numerical model will be illustrated by different applications in metal forming and impact simulations.

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A Multi-temporal Scale Approach using Extended Space-Time Finite Element Method

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Abstract

Many engineering applications are featured by a multitude of temporal scales that poses a great challenge for design and analysis. In this talk, we will address this important subject with the development of multi-temporal scale methods based on the integration of enrichment approach with space-time finite element method. Much of the work has been motivated by the pioneering efforts by Belytschko and co-workers [1] as well as Hughes et al [2]. We will demonstrate the applications in the areas of coupled atomistic/continuum simulation of nanomaterials [3] as well as simulation of high cycle fatigue failures with loading cycles on the orders of millions.

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Nanoscale Fracture in Graphene

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Abstract

Fracture of a monolayer graphene is governed by the competition between bond breaking and bond rotation at a crack tip. Using atomistic reaction pathway calculations [1], we identify a kinetically favorable fracture path that features an alternating sequence of bond rotation and bond breaking. Our results suggest that the mechanical cracking can create fracture edges with nanoscale morphologies due to the non-uniform bond deformation and rupture induced by the localized high stresses near the crack tip. Such fractured edges may provide a structural basis of tailoring the electronic properties of graphene either intrinsically or by further edge functionalization.

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Effects of surface elasticity and surface stresses in composites

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Abstract

It is well known that at the interface of dissimilar materials there exists a thin layer whose local elastic properties are different from those on either side of that interface and within which residual surface stresses (surface tension) are typically present. In composites both of those interface features influence the local stress and deformation fields, and they are likely to change response of a composite material to loading.

In this presentation the influence of surface elasticity and surface residual stresses on local elastic fields and on effective properties of composite materials will be discussed. The local elastic fields are responsible for initiation and propagation of damage, hence the interest in the influence of the interface properties on those fields. Overall properties of composites, on the other hand, are important in predicting mechanical behavior of sufficiently large composite structural systems.

For illustration, both of the above effects will be discussed in the context of unidirectional fiber reinforced composites. Specifically, two-dimensional problems in the plane perpendicular to those fibers, consisting of a cluster of inhomogeneities (which represent the cross sections of the fibers in the composite material at hand) embedded in an infinite homogeneous matrix, will be solved under various loading conditions using the boundary integral method. The interface between the fibers and the matrix will be described using Gurtin-Murdoch (1968) model. The stress distributions resulting from the interactions between the fibers will be shown to illustrate the influence of surface effects on the local elastic fields. The same solution will be used in conjunction with the Maxwell methodology to evaluate the effective properties of the composite represented by the cluster of fibers used in the analysis. The influence of surface effects on those properties will be discussed.

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Meshfree Methods: From Element-Free Galerkin to Maximum-Entropy Schemes

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Abstract

On introducing the Element-Free Galerkin (EFG) method [1] as a potentially attractive alternative to finite elements for many applications in solid mechanics, Ted Belytschko laid the foundations for what has come to be known as the area of *meshfree methods*. Emanating from his work in Reference [1], the mid- to late-1990s saw a surge in the development of many new meshfree methods to solve the continuum equations of solid continua. In EFG, as with many of the methods that initially followed, moving least squares (MLS) approximants were used. A method with different roots was the natural element method [2], which uses natural neighbor (Voronoi-based) interpolants. More recently, methods based on the principle of maximum-entropy [3, 4] have been proposed that provide a seamless connection from finite elements to meshfree approximations. In this talk, I will present some of the salient features and links between these meshfree methods, and in doing so, bring out how the initial ideas and impetus of Ted has led to the growth and advancement of meshfree methods.

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Quadrature techniques for enrichment functions in XFEM: Recent results on the Equivalent Polynomial approach

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Abstract

Current literature [1,2,3] shows an increasing interest on the quadrature of enrichment functions in the eXtended Finite Element Method. This interest is justified by both improving numerical efficiency and simplifying the computer implementation of the method.
One of the first approaches for dealing with the problem is based on equivalent polynomials [4]. The enrichment function, nonlinear and/or discontinuous, is replaced by a polynomial whose integral at the element level is equal to the one of the original function, allowing the straightforward use of standard Gauss quadrature.
The method is briefly illustrated and new results of its application will be shown, with some considerations related to its approximation properties compared to exact quadrature.

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A concurrent adaptive multiscale methodology for fracture in heterogeneous media

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Abstract

This presentation will introduce a concurrent adaptive multiscale methodology to handle situations in which both macroscopic and microscopic deformation fields strongly interact (e.g. near the tip of a crack). The method is based on the balance between numerical and homogenization error; while the first type of error states that elements should be refined in regions of high deformation gradients, the second implies that element size may not be smaller than a threshold determined by the size of the unit cell (UC) representing the material's microstructure. In this context, we build a finite element framework in which UCs can be embedded in continuum region through appropriate macro-micro boundary coupling conditions. By combining the idea of adaptive refinement with the embedded UC technique, the methodology ensures that appropriate descriptions of the material are used adequately, regardless of the severity of deformations. We will then show that our computational technique, in conjunction with the extended finite element method, is ideal to study the strong interactions between a crack and the microstructure of heterogeneous media. In particular, it enables an explicit description of microstructural features near the crack tip, while a computationally inexpensive coarse scale continuum description is used in the rest of the domain. The presentation will present several examples of crack propagation in materials with random microstructures and discuss the potential of the multiscale technique in relating microstructural details to material strength and toughness.

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A Spline Based Enrichment Function for Arbitrary Inclusions in XFEM with Applications to Finite Deformations

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Abstract

A novel enrichment function, which can model arbitrarily shaped inclusions within the framework of the extended finite element method (XFEM), is proposed. The internal boundary of an arbitrary shaped inclusion is first discretized, and a numerical enrichment function is constructed ``on the fly'' using spline interpolation. We consider a piecewise cubic spline which is constructed from seven localized discrete boundary points. The enrichment function is then determined by solving numerically a nonlinear equation which determines the distance from any point to the spline curve. Parametric convergence studies are carried out to show the accuracy of this approach compared to pointwise and linear segmentation of points, for the construction of the enrichment function in the case of simple inclusions and arbitrarily shaped inclusions in linear elasticity. Moreover, the viability of this approach is illustrated on a Neo-Hookean hyperelastic material with a hole undergoing large deformation. In this case, the enrichment is able to adapt to the deformation and effectively capture the correct response without remeshing.

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Multi-Scale and Multi-Physics Modeling of Proteins and Cells – A Computational Protocol for Complex Systems

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Abstract

Sickle cell anemia is one of the first diseases pinpointed to the genetic cause at the DNA level. Hemoglobin in its quaternary molecular structure is very much like a bead. The red blood cell has many such beads within the cell cytoskeleton. The cause of the sickle cell disease is a simple switch of the DNA base pair from A to T, with this switch, the codon will be changed from GAG to GTG. The normal hemoglobin at this particular location is slightly hydrophilic, thus tends to form a protective layer with the surrounding water molecules and is separated from each other. As a consequence, the normal red blood cell membrane is flexible and fluidic. Due to the sickle cell mutation, the hydrophilic spot becomes slightly hydrophobic and during the deoxygenated state, it tends to lose the protective layer of water molecules and consequently forms a chain of hemoglobin beads. Moreover, such chains will continue to form bundles and eventually yield a very stiff and sticky material property for the sickle cell membrane. In the end, these sickle cells tend to block the capillary vessels and cause the sickle cell anemia. In this research, we will use this well-established system as an example to explore a multi-scale and multi-physics modeling procedure for biological systems. We start with a series of molecular dynamics simulations of hemoglobin-hemoglobin interactions coupled with surrounding water molecules. Different level of coarse graining models will be employed to establish the likelihood of forming hemoglobin chains under difference circumstances. Simplified models of hemoglobin immersed in aqueous environment will be introduced in immersed boundary/continuum methods for the direct simulation of phase transitions of normal and sickle red blood cell membranes. Ultimately, cells modeled as soft continua will be coupled with viscous fluid in microcirculations. We hope that mathematical tools such as singular value decomposition, principal component analysis, coupled solution algorithm based on matrix-free Newton-Krylov iterative procedures introduced for such a complex fluid-solid system will help to establish a computational protocol for complex dynamical systems.

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An Efficient Augmented Finite Element Method (A-FEM) for Arbitrary Cracking and Crack Interaction in Solids

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Abstract

In this talk we shall present a new augmented finite element method (A-FEM) that can account for arbitrary, multiple intra-elemental discontinuities in solids without the need for extra DoFs as in the extended finite element method (X-FEM), or additional nodes as in the phantom node method (PNM). The A-FEM formulation employs four internal nodes to account for the crack displacements due to an intra-elemental weak or strong discontinuity and it permits repeated elemental augmentation to include multiple interactive cracks within a single element. It thus enables a unified treatment of damage evolution from a weak discontinuity to a strong discontinuity, and to multiple interactive cohesive cracks, all within a single element that employs standard external nodal DoFs only. WE shall also present a novel elemental condensation procedure that can solve the internal nodal DoFs as explicit functions of the nodal DoFs for any irreversible, piece-wise linear cohesive laws, which leads to a fully-condensed elemental equilibrium equation with mathematically exactness. The new A-FEM's high-fidelity simulation capabilities to interactive cohesive crack formation and propagation in homogeneous and heterogeneous solids will be demonstrated through several numerical examples. It will be shown that the proposed A-FEM, empowered by the new elemental condensation procedure, can achieve orders of magnitude improvement in numerical accuracy, efficiency and robustness, as compared to the X-FEM in a commercial code ABAQUS.

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The Extended Particle Difference Method for Solving Free Boundary Problems

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Abstract

In this study, an Extended Particle Difference Method(EPDM) for solving free boundary problems is proposed. The method is based on the meshfree strong formulation. To inherit attractive features of the Finite Difference Method and the Particle Method, it is equipped with the Moving-Least-Squares Derivative Approximation(MDA)[1] which is derived using Taylor series expanded by Moving Least Squares method. The EDPM is able to trace the topology change of free boundary since it employs neither grid structure for construction of approximation nor integral formulation that lessens merits of particle method; it effectively circumvents obstacles of the conventional particle method like the Element Free Galerkin method[2] in solving free boundary problems.
Partial differential equations for free boundary problem are directly discretized by a semi-explicit scheme. Time integration of the energy conservation equation is carried out by the Backward Euler scheme which is implicit but the update of topology change of free boundary is performed by an explicit scheme. Since the MDA already includes the kinetics relation of free boundary, the EPDM involve no additional interface evolving scheme like Level Set Method[3] which makes the total system nonlinear. Thus, assembling the difference equations yields a linear algebraic system. The excellence of the EPDM in accuracy and efficiency is clearly shown through various numerical experiments. The complicated topology change in 2-D domain is successfully simulated.

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In Situ Lithiation Mechanics of Silicon

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Abstract

Recent independent TEM studies evidenced highly anisotropic swelling and size-dependent fracture of silicon nanowires (SiNWs) upon lithiation. The origin of such anisotropic behavior and the underlying fracture mechanism remain elusive. Here, we develop a multiscale chemo-mechanical model to study the phase evolution, morphological changes, stress generation and fracture in lithiated SiNWs. The model couples the stress-dependent reaction-diffusion of lithium with the lithiation-induced elasto-plastic deformation. We show that the apparent anisotropic swelling is critically controlled by the orientation-dependent mobility of the atomically sharp phase boundary between the crystalline core and amorphous shell. The deformation anisotropy generates huge incompatible tensile strain (stress) in the outer lithiated shell, leading to the surface cracking of the SiNWs. Our modeling results agree strikingly well with the experimental data. The study sheds light on the lithiation-mediated degradation in nanostructured electrodes. The multiscale modeling framework is generic and provides a basis for simulating the morphological evolution, stress generation and fracture in high-capacity electrodes for the next-generation lithium-ion batteries.

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