IUTAM Symposium

Linking Scales in Computations:
From Microstructure to Macro-scale Properties

Agenda

DAY ONE: May 17, 2011

8:00-8:30 AM **Registration**

8:30-8:40 AM **Welcome and opening remarks**

Session: **Discrete-Continuum Modeling: I**
Chair: **Prof G. Z. Voyiadjis,** Louisiana State University, Baton Rouge, LA, USA

8:40 AM **Keynote**
J. Fish, Rensselaer Polytechnic Institute, Troy, NY, USA
Computational Continua[a]

9:20 AM
T. Junge**,** Ecole Polytechnique Fédérale de Lausanne, Switzerland
Linking discrete dislocations and molecular dynamics in 3D: A start[a]

9:50 AM
D. Moldovan, Louisiana State University, Baton Rouge, LA, USA
Hierarchical atomistic-mesoscale simulations of microstructure evolution and deformation in nanocrystalline materials[a]

10:20 AM **BREAK**

Session: **Discrete-Continuum Modeling: II**
Chair: **Prof F. Darve,** Laboratoire Sols, Solides, Structures – INPG, UJF, CNRS, Grenoble, France

10:35 AM **Keynote**
C. A. Duarte, University of Illinois at Urbana-Champaign, IL, USA
Bridging scales with a generalized finite element method[a]

11:15 AM
R. C. Picu, Rensselaer Polytechnic Institute, Troy, NY, USA
Coupled discrete-continuum models for mechanics problems in metals and polymers[a]

11:45 AM **Keynote**
A. Acharya, Carnegie Mellon University, Pittsburgh, PA, USA
Entropy of a constrained Hamiltonian system and mesoscale mechanics[a]

12:25 PM
H. M. Mourad, Los Alamos National Laboratory, Los Alamos, NM, USA
Interface-dominated behavior of multilayered metallic composites[a]

12:55 PM **LUNCH**

Session: **Discrete-Continuum Modeling: III**
Chair: **Prof. P. Van Houtte**

2:10 PM
J. Andrade, California Institute of Technology, Pasadena, CA, USA
Multi-scale modeling and characterization of granular matter: from grain kinematics to continuum mechanics[a]

2:40 PM **Keynote**
M. G. D. Geers, Eindhoven University of Technology, Eindhoven, Netherlands
Continuous-discontinuous scale transitions for localization in heterogeneous materials[a]

3:20 PM **BREAK**

3:35 PM **Keynote**
X. Chen, Columbia University, New York, NY, USA
Hierarchical modeling and simulation of mechanosensitive channels of large conductance[a]

4:15 PM **Keynote**
M. J. Buehler, Massachusetts Institute of Technology, Cambridge, MA, USA
Turning weakness to strength[a]

4:55 PM **Adjourn**

6:30 PM **Buses Depart Hotel**

7:00 PM – 9:00 PM
WELCOME BANQUET at NAVAL AVIATION MUSEUM

DAY TWO: May 18, 2011

Session: **Multi-scale Modeling of Deformation of Polycrystalline Materials: I**
Chair: **Dr. R. Lebensohn,** Los Alamos National Laboratory, Los Alamos, NM, USA.

8:30 AM **Keynote**

P. Suquet, Laboratoire de Mecanique et d'Acoustique, Marseille, France

Multi-scale modeling of the mechanical behaviour of polycrystalline ice[a]

9:10 AM **Keynote**

F. Roters, Max-Planck-Institut für Eisenforschung, Dusseldorf, Germany

A modular crystal plasticity framework applicable from component to single grain scale [a]

9:50 AM **BREAK**

Session: **Multi-scale Modeling of Deformation of Polycrystalline Materials: II**
Chair: **Prof. W. Brocks,** Kiel Technical University, Kiel, Germany

10:05 AM

A. J. Beaudoin, University of Illinois at Urbana-Champaign, USA

In-situ measurement of lattice strain and implications for continuum modeling of polycrystals [a]

10:35 AM **Keynote**

P. Van Houtte, Katholieke Universiteit, Leuven, Leuven, Belgium

Multi-scale modeling of the development of heterogeneous distributions of stress, strain, deformation texture and anisotropy in sheet metal forming [a]

11:15 AM

P. Franciosi, LPMTM, University Paris 13, Villetaneuse, France

Microstructure-based multi-laminate approaches of polycrystal plasticity[a]

11:45 AM

A. M. Habraken, Université de Liège, Liège, Belgium

'Smaller is softer' versus 'smaller is stronger' during the miniaturization of Nickel polycrystals: Experimental and numerical approaches[a]

12:15 PM

K. Inal, University of Waterloo, Waterloo, Canada

Numerical modeling of pure bending in aluminum alloys[a]

12:45 PM **LUNCH**

Session: **Multi-scale Modeling in Fluids**
Chair: **Dr. S. Balachandar,** University of Florida, Gainesville, FL, USA

2:00 PM **Keynote**
G. Karniadakis, Brown University & Massachusetts Institute of Technology, Cambridge, MA, USA
Dissipative particle dynamics and the triple-decker algorithm with applications to biomedical modeling[a]

2:40 PM
H. S. Udaykumar, University of Iowa, Iowa City, IA, USA
Multiscale modeling of shock interactions with heterogeneous materials[a]

3:10 PM
G. Jacobs, San Diego State University, San Diego, USA
Higher-order Eulerian-Lagrangian methods for shocked-particle-laden flow computation[a]

3:40 PM **BREAK**

Session: **Gradient Plasticity for Linking Scales**
Chair: **Dr. Martin Schmidt,** Air Force Research Laboratory, Eglin, FL, USA

3:55 PM **Keynote**
S. Ghosh, John Hopkins University, Baltimore, MD, USA
Temporal multi-scaling in image based crystal plasticity finite element modeling of dwell fatigue in polycrystalline titanium alloys[a]

4:35 PM **Keynote**
G. Z. Voyiadjis, Louisiana State University, Baton Rouge, LA, USA
Microstructure to macro-scale using gradient plasticity with temperature and rate dependent length scales[a]

5:15 PM **Adjourn**

6:45 PM **Vans depart Hotels for Banquet**

7:00 - 9:00 PM **Conference Banquet (Pensacola Beach)**

DAY THREE: May 19, 2011

Session: **Multi-scale Modeling of Damage and Failure in Polycrystalline Materials: I**
Chair: **Prof P. Suquet,** LMA-CNRS, Marseille, France

8:30 AM **Keynote**
R. Lebensohn, Los Alamos National Laboratory, Los Alamos, NM, USA
Modeling ductile damage of polycrystalline materials[a]

9:10 AM
R. Brenner, LPMTM, Villetaneuse, France
Numerical computation of the multifield coupling behaviour of composites using Fourier transform[a]

9:40 AM
S. V. Lomov, Katholieke Universiteit, Leuven, Leuven, Belgium
Damage initiation and development in textile composites: spanning nano - micro - meso - macro scales[a]

10:10 AM
O. Cazacu, University of Florida, Shalimar, FL, USA
Effects of the tension-compression asymmetry of the matrix on yielding of porous aggregates[a]

10:40 AM **BREAK**

Session: **Multi-scale Modeling of Damage and Failure in Polycrystalline Materials: II**
Chair: **Prof. A. Molinari,** Metz, France

10:55 AM **Keynote**
F. Darve, University Joseph Fourier, Grenoble, France
Second-order work, kinetic energy and failure[a]

11:35 AM **Keynote**
W. Brocks, Kiel Technical University, Kiel, Germany
Coupling aspects in the simulation of hydrogen-induced stress-corrosion cracking[a]

12:15 PM
N. Jacques, ENSIETA Bretagne, Brest, France
Microinertia effects on dynamic crack propagation in ductile materials[a]

12:45 PM **LUNCH**

Session: **Multi-scale Modeling of Damage and Failure in Polycrystalline Materials: III**
Chair: **Prof. A. Molinari,** University of Metz, Metz, France

2:00 PM **Keynote**
A. Combescure, INSA, Lyon, Villeurbanne, France
Ductile dynamic cracking from localization to initiation and propagation[a]

2:40 PM **Keynote**
A. Cuitino, Rutgers University, Rutgers, NY, USA
A concurrent multi-scale modeling and simulation strategy for confined granular solids[a]

3:20 PM
N. M. Cordero, Mines ParisTech, Evry, France
A third gradient theory to introduce the effect of the surface tension: applications to free surfaces, nano-wires and nanoporous materials[a]

3:50 PM **Adjourn**

Abstracts

SESSION: Discrete-Continuum Modeling: I

Computational continua

Jacob FISH

Multiscale Science and Engineering Center, Rensselaer Polytechnic Institute, Troy, NY 12180, USA

I present a new coarse-scale continuum formulation hereafter referred to as computational continua. By this approach the coarse-scale governing equations are stated on a so-called computational continua domain consisting of disjoint union of computational unit cells, positions of which are determined to reproduce the weak form of the governing equations on the fine scale. The label "computational" is conceived from both theoretical and computational considerations. From a theoretical point of view, the computational continua is endowed with fine-scale details; it introduces no scale separation; and makes no assumption about infinitesimally of the fine-scale structure. From computational point of view, the computational continua does not require higher order continuity; introduces no new degrees-of-freedom; and is free of higher order boundary conditions. The proposed continuum description features two building blocks: the nonlocal quadrature scheme and the coarse-scale stress function. The nonlocal quadrature scheme, which replaces the classical Gauss (local) quadrature, allows for nonlocal interactions to extend over finite neighborhoods and thus introduces nonlocality into the two-scale integrals employed in various homogenization theories. The coarse-scale stress function, which replaces the classical notion of coarse-scale stress being the average of fine-scale stresses, is constructed to express the governing equations in terms of coarse-scale fields only. Perhaps the most interesting finding of the present manuscript is that the coarse-scale continuum description that is consistent with an underlying fine-scale description depends on both the coarse-scale discretization and fine-scale details.

Linking discrete dislocations and molecular dynamics in 3D: a start

T. JUNGE[1], J.-F. MOLINARI[1], W.A. CURTIN[2], & T. NOGARET[2]

[1] *LSMS, Ecole Polytechnique Fédérale de Lausanne, Switzerland*
[2] *School of Engineering, Brown University, Providence, RI 02912 USA*

Many phenomena in crystalline metals such as friction, nano-indentation and ductile fracture are plasticity-driven and poorly understood. The physical complexity is further increased by the inherently multiscale nature of contact and fracture [Luan et al, 2005]. This study is aimed at a realistic numerical treatment of plasticity during nanoscale scratching of crystalline metal.

The principal mechanism of plasticity is dislocation nucleation and motion. Nucleation is an atomic nanoscale phenomenon and is often localised at interfaces, crack tips, etc., while dislocation motion is a microscale phenomenon occurring within grains in a polycrystalline microstructure [Swygenhoven et al, 2006]. The molecular dynamics (MD) method is able to accurately predict dislocation nucleation; however the time and length scale limitations [Berendsen, 2007] of MD do not permit for the description of the motion of entire dislocation networks. The latter are computed much more efficiently [Cai et al, 2003] with the discrete dislocation dynamics (DD) method where the details of the atomistic core are eliminated from consideration.

We present a method to extend to 3D the coupled atomistics and discrete dislocations (CADD) method [Miller et al, 2004; Shilkrot, 2004; Shilkrot et al, 2002]. To date, CADD has been restricted to plane strain problems with straight dislocations. In 3D CADD, the solid is split into two regions (e.g. Figure 1(a)): the MD region, where highly non-linear deformations (i.e. dislocation nucleation) and complex defect interactions are expected that require atomic resolution, and the DD region, where plastic behaviour due to dislocation motion can be computed at much lower cost. To couple these regions, the MD/DD interface (see Figure 1(b)) uses a layer in the MD region where approaching dislocations are detected and a layer in the DD region where fictitious pad atoms serve as boundary conditions for the MD region. An iterative solution permits for the tracking of dislocation lines that span the MD and DD regions, with minimal spurious forces due to the interface coupling. We apply the 3D coupling scheme to the simplest problem - motion of a straight edge dislocation under a uniform

applied shear. The results will be used to show capabilities and limitations of the method, and will guide the extension to more complex problems.

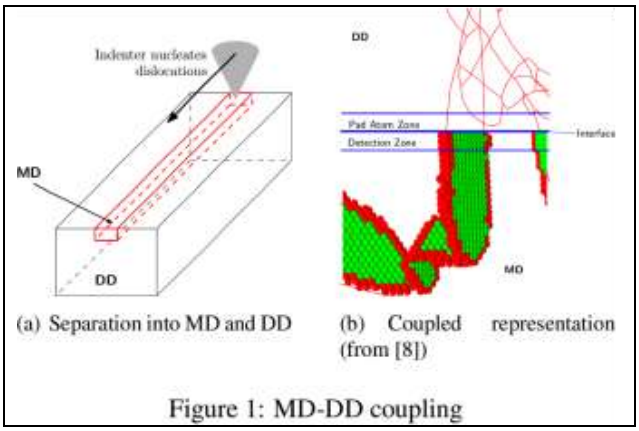

Figure 1: MD-DD coupling

Hierarchical atomistic-mesoscale simulations of microstructure evolution and deformation in nanocrystalline materials

Dorel MOLDOVAN

Department of Mechanical Engineering, Louisiana State University, Baton Rouge LA 70803, USA

There are two ingredients required to construct an efficient hierarchical multi-scale simulation model: first, one needs to acquire prior knowledge of the fundamental processes at the lowest scale involved, and second, it is necessary to develop a strategy for encompassing the lower-scale information into the coarser scales. To illustrate the implementation of the hierarchical approach, we present, in some detail, our molecular dynamics - mesoscale investigations of two phenomena in nanocrystalline materials: grain growth and grain-boundary controlled creep deformation.

Our molecular dynamics studies suggest that in nanocrystalline microstructures grain rotations play a complementary, equally important, role to grain growth by grain boundary migration. The presence of both grain-boundary migration and grain rotation introduces a physical length scale, Rc, into the system. The growth process is characterized by two regimes: if the average grain size is smaller than Rc, grain growth is grain-rotation dominated; by contrast, growth is dominated by grain-boundary migration for grain sizes greater than Rc. Our study reveals that the growth exponents are different for the two growth regimes. The combination of atomic-level with mesoscopic simulations based on the Needleman-Rice variational formalism for dissipative processes, enables the investigation of grain growth in systems containing a large number of grains and over long times.

Grain boundary diffusion and grain boundary sliding are the main plastic deformation mechanisms in fine-grained polycrystalline metals and ceramics at high homologous temperatures. By extending the variational functional approach, we investigate the deformation mechanism by grain-boundary diffusional creep (Coble creep) in polycrystalline materials. Mesoscopic simulations are used to elucidate the effects of grain size distribution and that of heterogeneity in grain boundary diffusivity and grain- boundary sliding resistance on creep deformation and stress concentration in polycrystals. Specifically, by using two-dimensional model microstructures we investigate the stress distribution around various topological and grain boundary inhomogeneities (i.e., distributions in grain boundary diffusivities and sliding resistances) at the onset of creep and during the steady state regime. Our simulations indicate that at higher strains the mechanism of grain boundary migration plays a critical role in mediating various topological transformations crucial for maintaining the equiaxed character of the microstructure.

SESSION: Discrete-Continuum Modeling: II

Bridging Scales with a Generalized Finite Element Method

C.A. DUARTE

Newmark Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

A major challenge in computational mechanics is the modeling of events in which sharply varying scales are present in a single system or phenomena. Predictive capability requires modeling multiscale phenomena simultaneously. The mathematical homogenization theory has been used extensively since the 1970s as a tool for analyzing multiscale response of materials. The method is based on the assumptions of spatial periodicity of microscale representative volume elements (RVE) and local uniformity of macroscale fields within each RVE [Ghosh et al, 2001]. The uniformity assumption is not appropriate in critical regions of high gradients, where the macroscale fields can vary considerably. Free edges, interfaces, macro cracks, neighborhoods of material discontinuities and, most importantly, in the regions of evolving microscale damage and instability are the potential sites of non-uniformity.

The generalized FEM (GFEM) is an instance of the partition of unity method which has its origins in the works of Babuška et al. [1994] and Duarte and Oden [1996]. The GFEM has been successfully applied to the simulation of dynamic propagating fractures, polycrystalline and fiber-reinforced microstructures, porous materials, etc. All these applications have relied on closed-form enrichment functions that are known to approximate well the physics of the problem. However, for many classes of problems–like those with material non-linearities or involving multiscale phenomena–enrichment functions with good approximation properties are not amenable to analytical derivation.

In this talk, we present a GFEM based on the solution of interdependent global (structural) and fine-scale or local problems. The local problems focus on the resolution of fine-scale features of the solution in the vicinity of, e.g., evolving fracture process zones while the global problem addresses the macro-scale structural behavior. Fine-scale solutions are accurately solved using an hp-adaptive GFEM and thus the proposed method does not rely on analytical solutions. These solutions are embedded into the global solution space using the partition of unity method. The boundary conditions for the fine-scale problems are provided by the available solution at a simulation step. The solutions of these problems are used, in turn, to build the GFEM solution space for the next simulation step. The proposed methodology enables accurate modeling of problems involving multiscale phenomena on meshes with elements that are orders of magnitude larger than those required by the FEM. This leads to considerable computational savings when compared with available methods for this class of problem. Numerical examples demonstrating the approximation properties of the proposed GFEM and its computational performance are presented.

Coupled Discrete-Continuum Models for Mechanics Problems in Metals and Polymers

R.C. PICU

Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA

This talk will review ongoing activities related to the development of multiscale methods for coupling discrete-discrete (coarse graining) and discrete-continuum models for the mechanics of a broad variety of materials with complex microstructure. Concurrent coupling of discrete and continuum models at zero Kelvin will be discussed first. An adaptive model selection procedure based on a set of error indicators is used to model a set of physical problems, including nanoindentation, fracture, and plastic deformation of a nano-porous material. In the context of the nano-porous material, a size effect is evidenced by which the yield stress depends not only on the pore volume fraction, but also on the pore size. An extension of this method to finite temperatures will be then presented. This is based on the partition of the phonon spectrum of the discrete region in a component which is treated in the continuum sub-domain as mechanical waves and another component which is treated as diffusive heat transport.

A sequential methodology for performing coarse graining in dense polymeric systems will be also discussed. This technique is aimed at reproducing the structure and the large scale dynamics of the fine scale (discrete) system using a coarse model (also discrete). Coarse scale potentials and coarse scale phase space constraints are defined and calibrated based on the dynamics and structure of the material at the fine, atomistic scale. The coarse model is then used to represent melts of mono- and poly-disperse polymers and nanocomposites.

Entropy of a constrained Hamiltonian system and mesoscale mechanics

Amit ACHARYA

Carnegie Mellon University, Pittsburgh, PA, 15213, USA

In classical equilibrium statistical mechanics, there is a formula for the entropy of a finite dimensional, constrained Hamiltonian system. It seems that this idea can be combined in a systematic way with space-time averaged, kinematically rigorous PDE models to produce mesoscale models physical phenomena. In doing so, the idea of 'local equilibrium' in non-equilibrium thermodynamics of extended systems can be given a specific operational meaning at the level of generating useful algorithms from it. The energetics and driving forces for dissipative mechanisms in these models can be precisely linked to atomistic behavior through well-defined, material-specific, one-time calculations that are expected to be possible on modern computers. This presentation will discuss the details of this formalism and illustrate it in the context of mesoscale dislocation plasticity.

Interface-dominated behavior of multilayered metallic composites

Hashem M. MOURAD

Los Alamos National Laboratory, MS B216, Los Alamos, NM, 87545, USA

We consider a multiscale modeling strategy for the behavior of composite materials consisting of alternating thin layers of two immiscible metals. Dislocations and other defects can be nucleated, annihilated, stored in or transmitted across the bi-metal interfaces in such composites. The effect of such interface-defect interactions on the macro-scale properties of the composite material is more pronounced when the thickness of individual layers is small, resulting in a high density of heterophase interfaces in the composite. In this interface-dominated regime, depending on their structure and properties, the bi-metal interfaces can endow their parent composite material with very desirable properties, e.g. outstanding damage resistance and significantly enhanced lifetimes, via their ability to mitigate damage accumulation induced under severe loading conditions. Metallic laminates with layer thicknesses in the sub-micron range can now be fabricated in bulk quantities (~ cm3) using severe plastic deformation processes, such as accumulative roll bonding [Rollett, 2009]. The proposed multiscale modeling strategy takes into consideration the structure of heterophase interfaces, and its evolution during the deformation process. This is crucial in elucidating the effect of interfaces on microstructural evolution under severe plastic deformation, with the goal of manipulating the fabrication process to produce composites with the desired properties.

SESSION: Discrete-Continuum Modeling: III

Multiscale modeling and characterization of granular matter: from grain kinematics to continuum mechanics

Jose ANDRADE

California Institute of Technology, Pasadena, CA, 91125, USA

Granular sands are characterized and modeled here by explicitly exploiting the discrete-continuum duality of granular matter. Grain- scale kinematics, obtained by shearing a sample under triaxial compression, are coupled with a recently proposed multiscale computational framework to model the behavior of the material without resorting to phenomenological evolution (hardening) laws. By doing this, complex material behavior is captured by extracting the evolution of key properties directly from the grain-scale mechanics and injecting it into a continuum description (e.g., elasto-plasticity). The effectiveness of the method is showcased by two examples: one linking discrete element computations with finite elements and another example linking a triaxial compression experiment using computed tomography and digital image correlation with finite element computation. In both cases, dilatancy and friction are used as the fundamental plastic variables and are obtained directly from the grain kinematics. In the case of the result linked to the experiment, the onset and evolution of a persistent shear band is modeled, showing-for the first time-3D multiscale results in the post-bifurcation regime with real materials and good quantitative agreement with experiments.

Continuous-discontinuous scale transitions for localization in heterogeneous materials

M.G.D. GEERS, E.W.C. COENEN, & V.G. KOUZNETSOVA

Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, Netherlands

Computational homogenization techniques are valuable approaches to assess the macroscopic behaviour of engineering materials on the basis of their underlying heterogeneous microstructure. At present, these techniques are being extended to address the ultimate mechanical state of the material, i.e. the transition from damage to fracture. The loss of separation of scales deserves particular attention to construct a multi-scale solution scheme that captures the gradual transition from a homogenized to a localized state of deformation. This is achieved with appropriate boundary conditions, averaging schemes, localization detection, and enriched kinematics.

This contribution focuses on the extension of computational homogenization schemes towards problems that involve damage, localization and fracture. Representative volume elements gradually evolve towards unique volume elements (i.e. the average solution depends on the local microstructural configuration), whereby homogenization cannot be applied anymore in the strict sense (the principle of separation of scales is violated). Within this context two categories of problems are addressed:

- Continuous-discontinuous multi-scale homogenization-localization approach for gradual localization in volume elements:
    - a solution for substructure periodic materials inspired by embedded localization bands.
    - a solution for more arbitrary heterogeneous materials capturing the onset of localization, the homogenization along an evolving localization band and the coupling to macroscopic discrete solution methods.
    - Computational homogenization of interfacial failure towards macroscopic cohesive zones using volumetric equivalent interface elements, preserving a representative nature of the material parallel to the interface.

Hierarchical modeling and simulation of mechanosensitive channels of large conductance

Xi CHEN

Department of Earth and Environmental Engineering, Columbia University, 500 W 120th Street, New York, NY 10027, USA

The gating pathways of mechanosensitive channels of large conductance (MscL) are studied using a molecular dynamics-decorated finite element method (MDeFEM). The phenomenological model treats transmembrane helices as elastic rods and the lipid membrane as an elastic sheet of finite thickness. The interactions between various continuum components are derived from atomistic energy calculations. Upon equi-biaxial tension, the structural variations along the gating pathway are consistent with previous analyses based on structural models and biased molecular-dynamics simulations. Detailed conformational changes and gating mechanisms of MscL when the membrane is under uniaxial/plane strain tension, bending, and torsion are also studied, as well as the interaction among neighboring proteins. In addition, the simulations of patch clamp and nanoindentation experiments are carried out. The MDeFEM framework offers a unique alternative to bridge detailed intermolecular interactions and biological processes occurring at large spatial and timescales. It is envisioned that such a hierarchical multiscale framework will find great value in the study of a variety of biological processes involving complex mechanical deformations such as muscle contraction and mechanotransduction.

Turning weakness to strength

Markus J. BUEHLER

Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave. Room 1-235A&B, Cambridge, MA, USA

Biology exquisitely creates hierarchical structures, where initiated at nano scales, are exhibited in macro or physiological multifunctional materials to provide structural support, force generation, catalytic properties, or energy conversion. This is exemplified in a broad range of biological materials such as hair, skin, bone, spider silk or cells. For instance, despite its simple building blocks spider silk is one of the strongest, most extensible and toughest biological

materials known, exceeding the properties of many engineered materials including steel. This is particularly puzzling since despite its great strength, spider silk is made of some of the weakest chemical bonds known, H-bonds. We have discovered that the great strength and extensibility of spider silk can be explained based on its particular structural makeup, which involves several hierarchical levels from the nano- to the macro-scale. Thereby, the structural confinement of H-bonds into ultra-small beta-sheet nanocrystals with dimensions of only a few nanometers is the key to overcome the intrinsic limitations of H-bonds, creating mechanically strong, tough and resilient cross-linking domains between a semi-amorphous phase composed of 3_1 protein helices (Keten, Buehler et al., Nature Materials, 2010). Our work unveils a material design strategy that enables silks to achieve superior material properties despite its simple and structurally inferior material constituents. Exploiting this concept could lead to a novel materials design paradigm, where enhanced functionality is not achieved using complex building blocks but rather through the utilization of universal repetitive constitutive elements arranged in hierarchical structures. We discuss analogies with other protein materials such as collagen and intermediate filaments, and present approaches towards the design of adaptable, mutable and active materials. Applications to the design of materials from mechanically inferior materials such as silica and silica are discussed.

SESSION: Multi-Scale Modeling of Deformation of Polycrystalline Materials: I

Multi-scale modeling of the mechanical behavior of polycrystalline ice

Claudiu BADULESCU, Renald BRENNER, Olivier CASTELNAU, Paul DUVAL, Fanny GRENNERAT, Noel LAHELLAC, Maurine MONTAGNAT, Hervé MOULINEC, Pierre SUQUET, & Quoc HUY VU

Mechanics and Acoustics Laboratory, Centre national de la recherche scientifique (CNRS), Marseille, France

Ice is an challenging material for understanding the overall behaviour of polycrystalline materials and more specifically the coupling between elastic and viscous effects during creep. At the single crystal level, ice is an hexagonal material with a rather mild elastic anisotropy but with a strong viscoplastic anisotropy. The strain-strain curve shows a softening behaviour depending on the strain-rate. The viscous anisotropy gives rise to the progressive development of intergranular and intragranular strain heterogeneities and to stress concentrations which are play an important role in the understanding of the creep behaviour of such materials.

The talk will report on the ongoing research of the group involved in the project on three different aspects of the problem. Full-field simulations based on a modification of the single crystal constitutive relations of Castelnau et al (2008) and a computational scheme based on FFT (Moulinec and Suquet, 1998, Lebensohn, 2001) are performed. They are used to assess the accuracy of a mean-field approach based on the notion of "effective internal variable" (Lahellec and Suquet, 2007). Finally, the statistics of the fields at the grain level obtained by the full-field approach and the mean-field approach will be compared to experimental characterization of intragranular strain heterogeneities (obtained by digital image correlation) on columnar specimens.

A modular crystal plasticity framework applicable from component to single grain scale

Franz ROTERS, Philip EISENLOHR, Denny D. TJAHJANTO, Christoph KORDS, & Dierk RAABE

Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

The solution of a continuum mechanical boundary value problem requires a constitutive response that connects deformation and stress at each material point. Such connection can be regarded as three separate hierarchical problems. At the top-most level, partitioning of the (mean) boundary values of the material point among its microstructural constituents and the associated homogenization of their response is required, provided there is more than one constituent present. Second, based on an elastoplastic decomposition of (finite strain) deformation, these responses follow from explicit or implicit time integration of the plastic deformation rate per constituent. Third, to establish the latter, a state variable-based constitutive law needs to be interrogated and its state updated. We demonstrate the versatility of such a modular framework, which has been implemented as a user subroutine into finite element packages, by considering three scenarios: Component-scale forming simulations comparing different homogenization schemes, selective refinement of the constitutive material description within a single geometry, and gradient-dominated deformation of an oligocrystalline patch using a non-local constitutive law.

SESSION: Multi-Scale Modeling of Deformation of Polycrystalline Materials: II

In-situ measurement of lattice strain and implications for continuum modeling of polycrystals

A. J. BEAUDOIN[1], K. HALM[1], M. OBSTALECKI[1], R. STORER[1], W. TAYON[2], & U. LIENERT[3]

[1] Department of Mechanical Science & Engineering, University of Illinois at Urbana-Champaign, IL, USA
[2] NASA, Langley Research Center, Hampton, VA 23681, USA
[3] Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

The technique of High Energy Diffraction Microscopy provides the capability to query crystallographic orientation and elastic strain within the sample volume of a polycrystalline material. Combined with in situ loading, data for the elasto-plastic transition on a grain-by-grain basis is accessible. That this data is for grains in a constrained environment -- not on the surface of the test specimen -- lends considerable value in assessing and advancing models for metal plasticity. In this presentation, experiments at the beamline 1-ID of the Advanced Photon Source of Argonne National Laboratory are reviewed. We then draw implications for models of polycrystal plasticity and damage evolution.

This work is supported by the NASA Marshall Flight Center through grant NNX09AN21G and Dept. of Energy grant DE-FG36-05GO15049.

Multi-scale modeling of the development of heterogeneous distributions of stress, strain, deformation texture and anisotropy in sheet metal forming

P. VAN HOUTTE[1], J. GAWAD[2], P. EYCKENS[1], B. VAN BAEL[1], Giovanni SAMAEY[2], & D. ROOSE[2]

[1] Department Metallurgy and Materials Engineering (MTM), Katholieke Universiteit, Leuven, Belgium
[2] Department of Computer Science, Katholieke Universiteit, Leuven, Belgium

Focus is on the implementation of texture-induced plastic anisotropy in FE simulations of metal forming. The crystallographic texture can be introduced as a state variable in every integration point. A multi-scale model is then called to calculate the stress-strain response and the local texture evolution in every integration point and for every strain increment. Less calculation-intensive is to use anisotropic analytical constitutive models, identified in advance from mechanical tests. These can also be done in a "virtual" way, i. e. using measured texture data and a multi-scale model. However, texture evolution is then not taken into account. An adaptive scheme for updating the texture and the anisotropy has been developed recently. Texture and anisotropy were updated by the ALAMEL-model. Results for some sheet metal forming processes are shown. The calculation times had been reduced from months to days. Predicted fields of plastic anisotropy and textures are discussed including experimental validation.

Microstructure-based multi-laminate approaches of polycrystal plasticity

P. FRANCIOSI

LPMTM, Université Paris 1, 99 av. Jean-Baptiste Clément, 93430, Villetaneuse, France

Plasticity of metals mainly involves, at the intra-granular scale, (multi-) planar slip possibly compensated by twinning mechanisms when available slip systems are not enough. The multi-slip activity is responsible for dislocation substructures inside the grains where basically dislocation-free cells are separated by dislocation “walls” which can also be seen as dislocations “carpets” with regard to a possibly parallel slip plane. The highly heterogeneous nature of the complex slip processes corresponds to a highly nonlinear plastic behaviour of the material. This calls for models capable of physically realistic simplification in order to provide reasonable estimates of effective behaviour in avoiding excessive machinery. Among tentative models, laminate-based ones have been shown relevant to catch the main features of slip heterogeneity, allowing the possibility of accounting for both those coming from intra-crystalline dislocation substructures and those related with trans-crystalline interactions. Furthermore, with regard to the homogenization framework based on mean field approximations at the scale of the material “phases”, it is known that laminate layers are sub-domains where plasticity can be considered as almost everywhere homogeneous, so allowing the quite simple use of the Transformation Field Analysis (TFA) to estimate the overall behaviour.

We here discuss different possible laminate-based descriptions of single and poly-crystal plasticity (rank-n laminate structures and laminate systems namely, differently describing the slip arrangement), some of which have been previously introduced and examined in various contexts, with the goal of selecting the simplest relevant schemes. If all laminate-based descriptions of poly-crystal plasticity are compatible with the use of a TFA approach (of the most efficient non uniform NTFA type), they also are compatible with other homogenization models, provided some additional complexity. It is also reminded how the use of a regularized Schmid-like plastic flow criterion up to the poly-crystal level can simplify the scale connection between this local modeling of plasticity and subsequent computational simulations on structures.

'Smaller is softer' versus 'smaller is stronger' during the miniaturization of nickel polycrystals: experimental and numerical approaches

Clément KELLER[1], Laurent DUCHÊNE[1], Eric HUG[2], & Anne-Marie HABRAKEN[1]

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The strong trend of miniaturization of metallic parts used in micro-devices such as MEMS (Micro-Electro-Mechanical Systems) motivated the material science community to understand the deformation mechanisms at small scales. During the miniaturization, the transition from the polycrystal scale (macroscopic) to the multi-crystal scale (a few grains along the shortest dimension of the metallic parts), or to the quasi-single crystal scale (one grain along the shortest dimension) significantly modifies the material mechanical behavior involving reliability and forming issues. The results presented here are focused on the analysis and the understanding of the mechanical properties of high purity polycrystalline nickel with different grain sizes and thicknesses submitted to a tensile deformation.

The scale transition was first characterized experimentally. Tensile test experiments were carried out on nickel samples of controlled microstructure (no crystallographycal texture, same grain size distribution and grain boundaries character) with thicknesses ranging from 12.5 µm to 3.2 mm. The thickness reduction induced a large modification of the mechanical behavior triggered by the number of grains across the thickness.

A strain gradient crystal plasticity model implemented in a finite element code was then investigated to simulate the same tensile tests on Nickel polycrystals. The effect of the miniaturization can be taken into account in the model thanks to an internal length scale linked to the material structure, i.e. the length of the Burgers vector. Besides, the stress and strain gradients inside the different grains (due to the presence of e.g. grain boundaries, free surfaces…) are accommodated by the geometrically necessary dislocations. The material parameters for this model were identified on nickel single crystals submitted to tensile tests along different directions.

The analysis of the numerical results, supported by the experimental observations for new loading conditions (shear test, plane strain test) permitted to understand the deformation mechanisms taking place during plastic straining at the different sample scales. Applications toward microforming are studied thanks to collaborations with Galati university and SIMtech in Singapore.

Numerical modeling of pure bending in aluminum alloys

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A new three-dimensional (3D) finite element analyses based on rate-dependent crystal plasticity theory has been developed to investigate pure bending in aluminum alloys. The new model can incorporate electron backscatter diffraction (EBSD) maps into finite element analyses. The numerical analysis not only accounts for crystallographic texture (and its evolution) but also accounts for 3D grain morphologies since a 3D microstructure (constructed from two-dimensional EBSD data) has been employed in the simulations. A unit cube (numerical model for three dimensions) approach has been adopted where an element or number of elements of the finite element mesh are considered to represent a single crystal within the polycrystal aggregate. Numerical simulations of pure bending have been performed for various aluminum alloys. The effects of grain sizes and morphologies on localized deformation and surface topography (roughness) are investigated. Furthermore, a multi-scale approach (special finite elements) is presented to investigate the contribution of grain boundaries on the inhomogeneous strain partitioning during pure bending.

SESSION: Multi-Scale Modeling in Fluids

Dissipative particle dynamics and the triple-decker algorithm with applications to biomedical modeling

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We present a hybrid method based on coupling the Molecular Dynamics (MD) method, the Dissipative Particle Dynamics (DPD) method, and the incompressible Navier-Stokes (NS) equations. MD, DPD and NS are formulated in separate sub-domains and are coupled via an overlapping region by communicating state information at the sub-domain boundaries. Imposition of boundary conditions in the MD and DPD systems involves particle insertion and deletion, specular wall reflection and body force terms. The latter includes a boundary pressure force in order to minimize near-boundary density fluctuations, and an adaptive shear force which enforces the tangential velocity component of boundary conditions. The triple-decker algorithm is verified for prototype flows, including simple and multi-layer fluids. Biomedical applications including multiscale modeling of hematologic disorders will also be discussed.

Multi-scale modeling of shock interaction with heterogeneous materials

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Interactions of shocks with heterogeneous materials can play a role in the dynamics of several systems, including dusty gases, energetic materials such as plastic bonded explosives, geological materials etc. In these systems, while the large scale dynamics of the system is often described by continuum mixture theories of the Baer-Nunziato type, such formulations rely on closure models which are typically drawn from empirical observations. An alternate route to obtaining closure models is through direct numerical simulations of the subgrid-scale phenomena. This work presents an approach to construct such subgrid- (meso-) scale models by performing detailed computations with resolved particulate phases. As a first example, the dynamics of a particle-laden gas in shocked flows is simulated; this system involves multi-scale effects derived from the micro- (i.e. particle) scale interactions that govern the overall (macro-scale) evolution of the mixture. Data on the forces experienced by particles in a cloud are collected from DNS using a compressible Eulerian-Lagrangian solver and provided to an artificial neural network (ANN); the simulations are performed for a range of control parameters, such as Mach number, particle radii, particle-fluid density ratio, position, and volume fraction. Beginning with a simple single stationary particle case and progressing to moving particle laden clouds, the ANN is able to evolve and reproduce correlations between the control parameters and particle dynamics. The trained ANN is then used in computing the macro-scale flow behavior in a model of shocked dusty gas advection. The model predicts particle motion and other macro-scale phenomena in agreement with experimental observations. As a second example the meso-scale dynamics of a porous explosive is simulated to capture the effects of energy localization at hot spots, an important subgrid-scale mechanism for the initiation of detonation in heterogeneous energetic material. Here the interaction of shocks with a distribution of voids is studied and a sub-grid scale model for the hot spot effect on initiation is examined. Results on void-void interactions will be presented.

Higher-order Eulerian-Lagrangian methods for shocked-particle-laden flow computation

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[2] *Department of Mathematics, Hong Kong Baptist University, Hong Kong, China*

In this talk, we will discuss the developments and validation of an efficient high-resolution scheme for solution of shocked flows with small scale flow features that are laden with particles and droplets. These flows are of critical relevance to technologies such as fuel injectors in scramjets and dust explosions.

Computation of these flows that exhibit a wide range of scales has proven to put heavy demands on computational models and methods. We consider the Eulerian-Lagrangian (EL) or particle-mesh method that is prevalent for the solution of particle-laden turbulent flows. In these methods a continuum flow model (usually Navier-Stokes) is approximated in the Eulerian frame on a static mesh, whereas individual particles are traced in the Lagrangian frame based on the kinematic equations and Newton's second law. The treatment of particles as volumeless mathematical points in EL economizes the tracing of particles, and makes the simulation of large number of particles, typical of any realistic industrial flow feasible. EL methods suffer from a plethora of errors including diffusion, dispersion, coupling and dispersion errors, particularly when shocks capturing is required. These errors are now showing up as bottleneck in widely used low-order particle-mesh methods with large diffusion and dispersion errors.

We discuss the development of a particle-mesh algorithm (also known as an Eulerian-Lagrangian method) based on a high-order WENO-spectral and WENO-Central Difference Navier-Stokes solver for computation of particle-laden flows with shocks. The WENO-spectral based particle-mesh has the potential to combine excellent shock capturing and accurate solution of small scale flow features and particle physics with computational efficiency. We will present the developments of high-order coupling approaches of the particle solver to the Euler spectral solver and the development of a Hybrid WENO-Central Difference Navier-Stokes solver for two-phase flows. We will also discuss validation of the computation against experiments of particle-laden shocked flows in shock tubes and of cross stream air and ethylene flow injection in supersonic air flows.

SESSION: Gradient Plasticity for Linking Scales

Temporal multi-scaling in image based crystal plasticity finite element modeling of dwell fatigue in polycrystalline Ti alloys

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The recent years have seen a paradigm shift towards the use of material microstructure based detailed mechanistic models for predicting fatigue crack nucleation and propagation. These approaches seek accurate description of material behavior through crystal plasticity based finite element models. This talk will present the development of a microstructure based modeling of dwell fatigue crack initiation in polycrystalline alloy Ti alloys. Local stress peaks due to load shedding from time dependent plastic deformation fields in neighboring grains are responsible for crack initiation in dwell fatigue. The model implements crystal plasticity theory with explicit grain structures, and the mechanical response of polycrystalline aggregates are deduced from the behavior of constituent crystal grains. Finite element calculations show that depending on the loading conditions, significant gradients of stresses or strains can evolve, even within a single slip system. These calculations provide a platform for the implementation of physics based crack nucleation and propagation criterion that accounts for the effects of microstructural inhomogeneity. Systematic development of a crystal plasticity based fatigue crack nucleation model for titanium alloys under dwell loading is conducted in this study.

A major bottleneck with 3D crystal plasticity finite element (CPFE) simulations for fatigue life prediction is the accommodation of large number of cycles to failure, often observed in experiments. In single time-scale CPFE solutions using conventional time integration algorithms, each cycle is resolved into a large number of time steps. A high time step resolution is required for each cycle throughout the loading process, often leading to prohibitively large computational requirements. The presentation will discuss a wavelet transformation based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations. The WATMUS algorithm does not require any scale-separation and naturally transforms the coarse time scale response into a monotonic cycle scale without the requirement of sub-cycle resolution. The method significantly enhances the computational efficiency in comparison with conventional single time scale integration methods. Adaptivity conditions are also developed for this algorithm to improve accuracy and efficiency.

Second order work, kinetic energy and failure

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Failure is usually viewed as the consequence of the existence of some limit stress states, which cannot be trespassed by the material. However the experiments on geomaterials show that some failure states can be reached largely before the plastic limit condition for some loading paths with a mixed control (i.e. stress-strain control). The most known example is probably the undrained triaxial compressions axially force controlled on loose sands [Daouadji et al., 2010].

The origin of this unusual behaviour lies in the strong non-associativeness of geomaterials, which implies the non-symmetry of the elasto-plastic matrix. If so, the second order work criterion (non-definite positiveness of the constitutive matrix) can be fulfilled before the plastic limit surface, the corresponding mechanical states belonging to a bifurcation domain. The basic link between the existence of some limit states, the loss of positiveness of the constitutive matrix and the burst of kinetic energy at failure is shown theoretically [Nicot et al., 2009]. The equations of the boundaries of the bifurcation domain and of the instability cones in 3D (gathering the potentially unstable loading directions) are established [Prunier et al., 2009]. Eventually these failure modes are observed in direct numerical modeling by a discrete element model [Sibille et al., 2007]. The existence of a bifurcation domain, of instability cones and the necessity of mixed loading conditions for an effective failure are discussed. Some features of these failure modes are also exhibited from these results.

SESSION: Multi-Scale Modeling of Damage and Failure in Polycrystalline Materials: I

Modeling ductile damage of polycrystalline materials

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In this lecture we will present a new constitutive model for polycrystalline materials with intergranular cavities based on homogenization and test it against full-field numerical simulations. Such materials are prevalent in many engineering applications (e.g., forming of materials with initial porosity, spallation of metals under dynamic loading conditions, etc), where the dilatational effects associated with the presence of cavities must be accounted for, and standard polycrystalline models for incompressible plasticity are not appropriate. On the other hand, it is not clear that the use of porous plasticity models with isotropic matrix behavior is adequate, particularly, when large deformations can lead to texture evolution resulting in marked matrix anisotropy, and also to significant changes in pore shape, resulting in additional anisotropy development. In this work, we make use of state-of-the-art homogenization [Liu et al., 2004] to develop constitutive models simultaneously accounting for texture of the matrix, porosity and pore shape and orientation. The predictions of the models are compared with full-field numerical simulations based on Fast Fourier transforms [Michel et al., 2000] to study the influence of different microstructural features (e.g. overall porosity, texture of the matrix phase, single-crystal anisotropy, etc.) and type of loading (triaxiality) on the dilatational viscoplastic behavior of voided polycrystals [Lebensohn et al., 2011]. The results are also compared with the predictions of isotropic-matrix porous plasticity models to assess the effect of the possible matrix anisotropy in textured samples.

Numerical computation of the multifield coupling behaviour of composites using Fourier transform

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A numerical homogenization scheme based on Fourier transform is applied to investigate the effective response as well as the local fields which take place within smart composite materials which exhibit a multifield coupling constitutive relation. It consists in the iterative resolution of coupled Lippmann-Schwinger equations for a periodic microstructure discretized on a regular grid. A simple scheme relying on the Green operators for the related uncoupled properties (elasticity, permittivity, conductivity etc.) and valid for an arbitrary contrast on the constituents properties is presented. The results are compared in various coupling and microstructural situations with analytical and finite element results.

Damage initiation and development in textile composites: spanning nano – micro – meso – macro scales

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Damage response of fibre reinforced composites to loading is defined by the hierarchical structure of the composite material, which spans several structural and scale levels, from macro (composite part), via meso (yarn organization in the textile reinforcement) and micro (fibrous structure of the yarns) down to nano (nano-scale additives to the resin) and covers nine decimal orders of magnitude in length scale (from 100 m to 10-9 m). The paper presents an overview of models, describing initiation and development of damage and loss of load-carrying ability of fibre reinforced composites, which take into account this hierarchical organisation and have as a starting point mathematical description of the internal geometry of the composite on different structural levels. A sequence of damage criteria and damage propagation models are constructed:

- Macro-level: criterion of failure of textile composite, linked to different stages of micro/meso-level damage initiation/propagation, to be used in structural analysis;
- Meso-level: finite element model of unit cell of textile composite; criterion of damage initiation; local and non-local models of degradation of load-carrying capability;
- Micro-level: prediction of damage initiation based on properties of matrix and fibres; fracture mechanics analysis of stress shielding in the presence of cracks on fibre/matrix interface;
- Nano-level: redistribution of stress concentration between the micro- and nano-scale, delay of the damage initiation and increase of toughness of the material.

The models are discussed in conjunction with experimental evidence on different scale/structural levels.

Effects of the tension-compression asymmetry of the matrix on yielding of porous aggregates

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A significant strength differential effect (different behavior 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 yielding, description of damage by void growth in such materials remains a challenge.

In this talk are presented, new plastic potentials for isotropic and anisotropic porous materials containing spherical voids randomly distributed in a matrix displaying tension-compression asymmetry. These analytic potentials are derived using Hill-Mandel non-linear homogenization techniques. Cazacu et al.'s (2006) yield criterion is used to characterize the yield and flow of the incompressible matrix. The isotropic analytic potential developed depends on all stress invariants of stress. It predicts the exact solution of a hollow sphere loaded in hydrostatic tension or compression. Furthermore, it is shown that it reduces to Gurson's (1977) criterion in the case when the matrix material has the same yield in tension and compression. The anisotropic plastic potential developed depends on all the invariants of stress and mixed stress-anisotropy invariants. It reduces to Benzerga and Besson (2001) criterion, if the matrix material is transversely isotropic and has no strength differential effects. The accuracy of these analytical criteria is assessed through comparison with finite-element cell

calculations. Finally, an elastic-plastic damage model with yielding described by the developed criteria is presented. Single-element tests illustrate the salient features of this model. Simulation results of necking in a tensile test show that if the compressive strength of the matrix is lower than its tensile strength, void growth and damage expansion is restricted.

SESSION: Multi-Scale Modeling of Damage and Failure in Polycrystalline Materials: II

Microstructure to macro-scale using gradient plasticity with temperature and rate dependent length scales

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Classical continuum plasticity does not incorporate material length scales ℓ and it is not able to predict the size dependency. The finite element analysis based on this kind of models suffers mesh dependency and mesh sensitivity in the case of problems involving strain localization and instability. However, strain gradient plasticity (i.e. Fleck and Hutchinson 1997; Bammann et al. 1999; Voyiadjis et al. 2001) which is based on introducing the gradient in the constitutive relationships has been able to account for the micro-structural interaction, in order to improve the accuracy of the finite element analysis. One major issue in strain gradient plasticity is the determination of the material intrinsic length scale ℓ that scales with strain gradient using stress-strain behavior from macroscopic scale as well as information from micromechanical tests.

In this work, following the Nix and Gao (1998) approach, the gradient theory and crystal plasticity is used to derive expressions that describe the hardness as a function of indentation depth which accounts for various temperatures and strain rates (TRISE). The developed TRISE model is also able to capture the local hardening effect in polycrystalline metals trough inclusion of the effect of grain boundary in the hardness behavior. Combining this expression with the outcomes of nano-indentation experiments of a material allows one to determining the variable material intrinsic length scale ℓ. The aforementioned approach is used to determine the length scale of various fcc and bcc metals in different, rate, temperature, and grain size.

Furthermore, a general framework for the analysis of heterogeneous media that assesses a strong coupling between viscoplasticity and anisotropic viscodamage evolution is formulated within the framework of thermodynamic laws and nonlinear continuum mechanics. The proposed formulations include thermo-elastic-viscoplasticity with anisotropic thermo-elastic-viscodamage, a physically based viscoplastic (rate and temperature dependent) and a dynamic viscodamage criterion, the associated flow rules, non-linear strain hardening, strain-rate hardening, and temperature softening. The evolution laws are impeded in a finite deformation framework based on the multiplicative decomposition of the deformation gradient into elastic, viscoplastic, and viscodamage part. The aforementioned non-local constitutive model is implemented into the ABAQUS as a user material code. Along with the variable length scale obtained for different metals through nanoindentation experiments, this constitutive model is used for modeling impact damage.

Coupling aspects in the simulation of hydrogen-induced stress-corrosion cracking

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Modeling of hydrogen-induced stress-corrosion cracking (HISCC) has to consider coupling effects between the mechanical and the diffusion field quantities. Four main topics are addressed: i) surface kinetics, ii) diffusion, iii) deformation and iv) crack growth. Surface kinetics is realised by a chemisorptions model, hydrogen diffusion is formulated by an enhanced diffusion equation including effects of plastic deformation, deformation rate and hydrostatic pressure, deformation is described by von Mises plasticity, and crack growth is simulated by a cohesive model, where both yield and cohesive strength depend on the hydrogen concentration. The effect of atomic hydrogen on the local yield strength is modelled by the so-called HELP (Hydrogen-Enhanced Localised Plasticity) approach, and the influence on the cohesive strength is taken into account by the so-called HEDE (Hydrogen-Enhanced DEcohesion) model. As the two models predict contrary effects of atomic hydrogen on the material behaviour, namely a decrease of the local yield strength resulting in larger plastic deformations and a reduction of the cohesive strength and energy inducing lower ductility, respectively, the coupling phenomena are studied in detail. The model is verified by comparing experimentally measured and numerically simulated CTOD R-curves of C(T) specimens.

Microinertia effects on dynamic crack propagation in ductile materials

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Dynamic fracture is an important issue in a number of industrial applications. For example, understanding dynamic crack propagation and arrest is mandatory for the evaluation of the integrity of aircraft structures, pipelines and nuclear pressure vessels.

Ductile fracture is the result of initiation, growth and coalescence of voids in the material. At elevated strain rate, large velocities and accelerations are present in the vicinity of the void surface inside the matrix material. Recently, it has been shown that microinertia effects are significant when dealing with plate impact experiments, see Jacques et al (2010). There are only few studies investigating the role of micro-inertia in dynamic ductile crack growth. Glennie (1972) proposed a simple analytical model for void growth in the vicinity of a blunted crack tip in which the effect of micro-inertia is taken into account. In the model of Glennie (1972), the effect of damage due to void growth on the stress state in the vicinity of the crack tip is neglected. Nevertheless, it has been shown that the inertial resistance to void expansion limits the speed at which cracks can propagate.

A constitutive damage model of a porous plastic material taking micro inertia into account is proposed. Micro-inertia effects are incorporated according to the dynamic homogenization method proposed by Molinari and Mercier (2001). Material rate dependence and adiabatic heating are also accounted for in the present analysis. The proposed material model has been implemented in a finite element code. The fracture of an axisymmetric notched bar and of a double edge cracked specimen is investigated. In both cases, the influence of micro-inertia is found to be significant. Because micro-inertia prevents damage to develop too rapidly, a regularizing effect is observed which reduces the mesh sensitivity of the simulations. Micro-inertia is also found to lead to lower crack speed and higher fracture toughness, compared to situation where this contribution is neglected.

SESSION: Multi-Scale Modeling of Damage and Failure in Polycrystalline Materials: III

Ductile dynamic cracking from localization to initiation and propagation

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This presentation is devoted to the prediction of crack initiation and propagation with X-FEM. Two main points shall be developed. The first point is a simple and efficient way to model damage cracking transition: it will be shown how one can predict the appearance of a crack in a fragile or ductile damaging material. The case of a micro structurally long crack will be presented. A strategy to switch from a localizing damage model to an energy equivalent cohesive zone model shall be presented. This cohesive law is then inserted in an X-FEM framework. Examples of application to crack propagation in ductile regime shall be presented and compared to experimental results. The second one dedicated to the prediction of dynamic crack propagation in case of ductile cracking. It will be shown how a simple model can predict in the same framework ductile brittle transition: this simple model shall be applied to Kalthoff brittle ductile transition experiments.

A concurrent multi-scale modeling and simulation strategy for confined granular solids

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A modeling and simulation strategy for the predicting the behavior of granular solids is described in this talk. The strategy hinges on a concurrent description of granular systems where a discrete representation of the each individual particle is merged with a continuum level formulation. This approach has the ability to predict macroscopic behavior (system level) based on microscopic properties (particle level), rendering continuum-level constitutive models unnecessary. The effective mechanical response accounts for point-to-point variations due particle level heterogeneities and particle distributions. In addition, this approach is amenable for describing the process of inter-particle bonding which is responsible for key performance characteristics of the compacted solid as such as strength, friability, disintegration and dissolution.

A third gradient theory to introduce the effect of the surface tension: applications to free surfaces, nano-wires and nanoporous materials

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Due to their different local environments, atoms at a free surface and in the bulk of a material have different energies. The difference between these energies, the so-called surface free energy, is responsible for surface tension. As the free surface region is only a few atomic layers thin, the effect of the surface tension can be neglected when the material microstructure exhibits characteristic lengths in the micrometer range or larger. However, in the case of nano-sized materials, the ratio between the surface and the volume is much greater and hence the surface region behaviour can no longer be neglected.

There are several ways to introduce the mechanical properties of the surface or interface. If an interface separating two homogeneous bulk phases is considered, the interfacial properties can be defined by assuming that the interphase has a finite volume so that its thermodynamic properties can be assigned in the usual way [Capolungo et al, 2005]. Three phases are present in this approach and the interphase boundaries may be defined more or less arbitrarily. One can also consider that the two homogeneous phases are separated by a single dividing surface; the thermodynamic properties of the interface can then be defined as the excess over the values obtained for both bulk phases separated by a zero-thickness surface [Dingreville et al, 2005].

We propose to introduce the effect of the surface tension with a continuous method that does not distinguish the properties of the surface/interfaces from the bulk behaviour [Germain, 1973]. R.D. Mindlin showed [1965] that the third gradient of displacement is necessary to introduce a cohesion modulus from which surface tension will arise in an isotropic elastic medium. Here, the need to have such a higher order theory in a recent paper [Forest et al, 2010] is discussed and the work of Mindlin is compared with more recent developments, such as those reported in [Casal, 1973].

The method will be validated in the simple case of a free surface for which an analytical solution for the displacement of atoms from the surface when a bulk crystal is cut into two pieces is known. Then, a finite element implementation of the model will be proposed based on the micromorphic approach [Forest, 2009] and less trivial cases such as nano-wires [Agrawal et al, 2008] or nanoporous materials [Duan et al, 2005] will be considered. In particular, the higher order moduli responsible for the apparent stiffening or softening of elastic properties of the nano-wire will be shown. Finally, results from periodic homogenisation applied to third gradient media to predict the size-dependent effective properties of some nano-porous materials will be presented.

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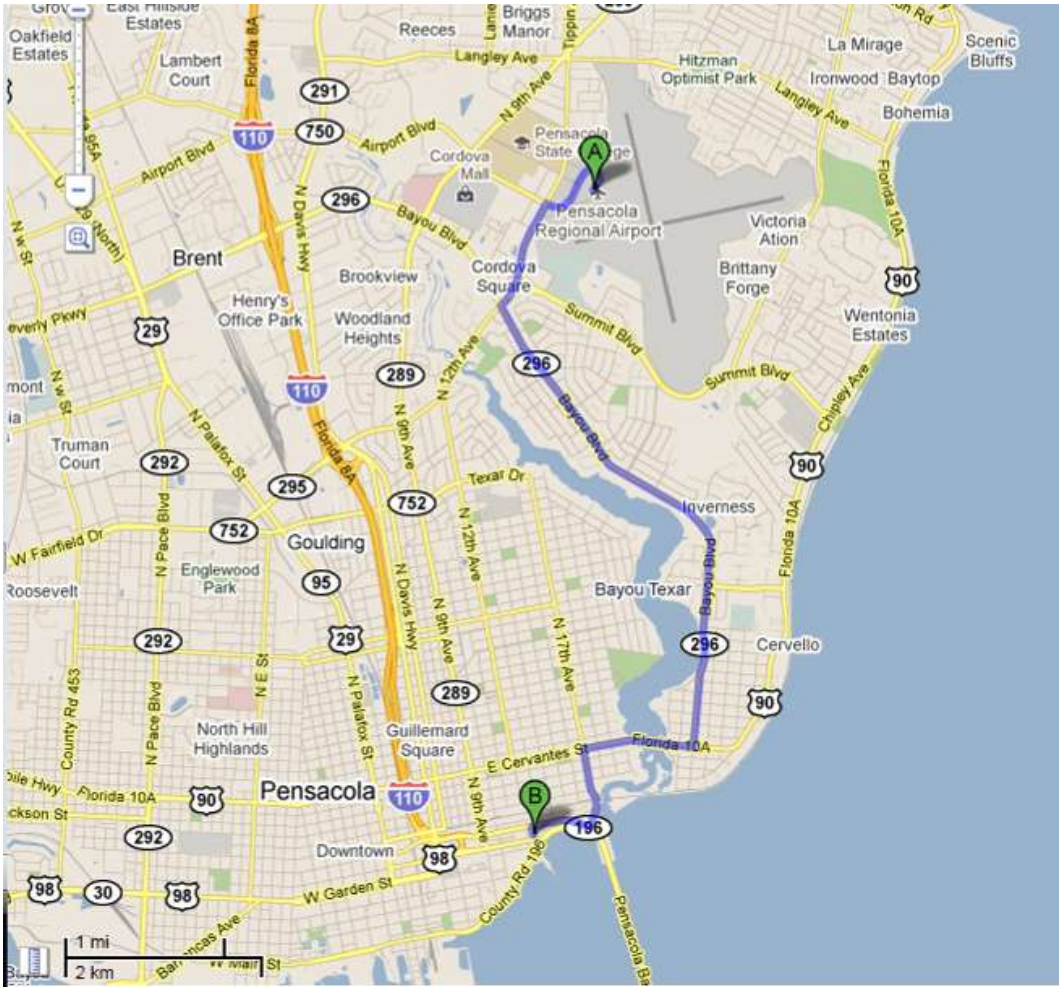
Directions & Maps

Driving from Pensacola Regional Airport (PNS) to Courtyard Pensacola Downtown

FROM: Pensacola Regional Airport (PNS)
GPS: N 30.47629 W 87.19399

1. Head northeast on Airport Blvd	0.4 mi
2. Slight right to stay on Airport Blvd	0.1 mi
3. Turn left at N 12th Ave	0.7 mi
4. Turn left at Bayou Blvd	2.9 mi
5. Slight left at Perry Ave	0.5 mi
6. Turn right at E Cervantes St	0.7 mi
7. Turn left at the 3rd cross street onto N 17th Ave	0.5 mi
8. Turn right at E Gregory St	0.4 mi
9. Hotel on left	

TO: Courtyard Pensacola Downtown
700 E Chase Street
Pensacola, FL 32502
GPS: N 30.41687 W 87.20051

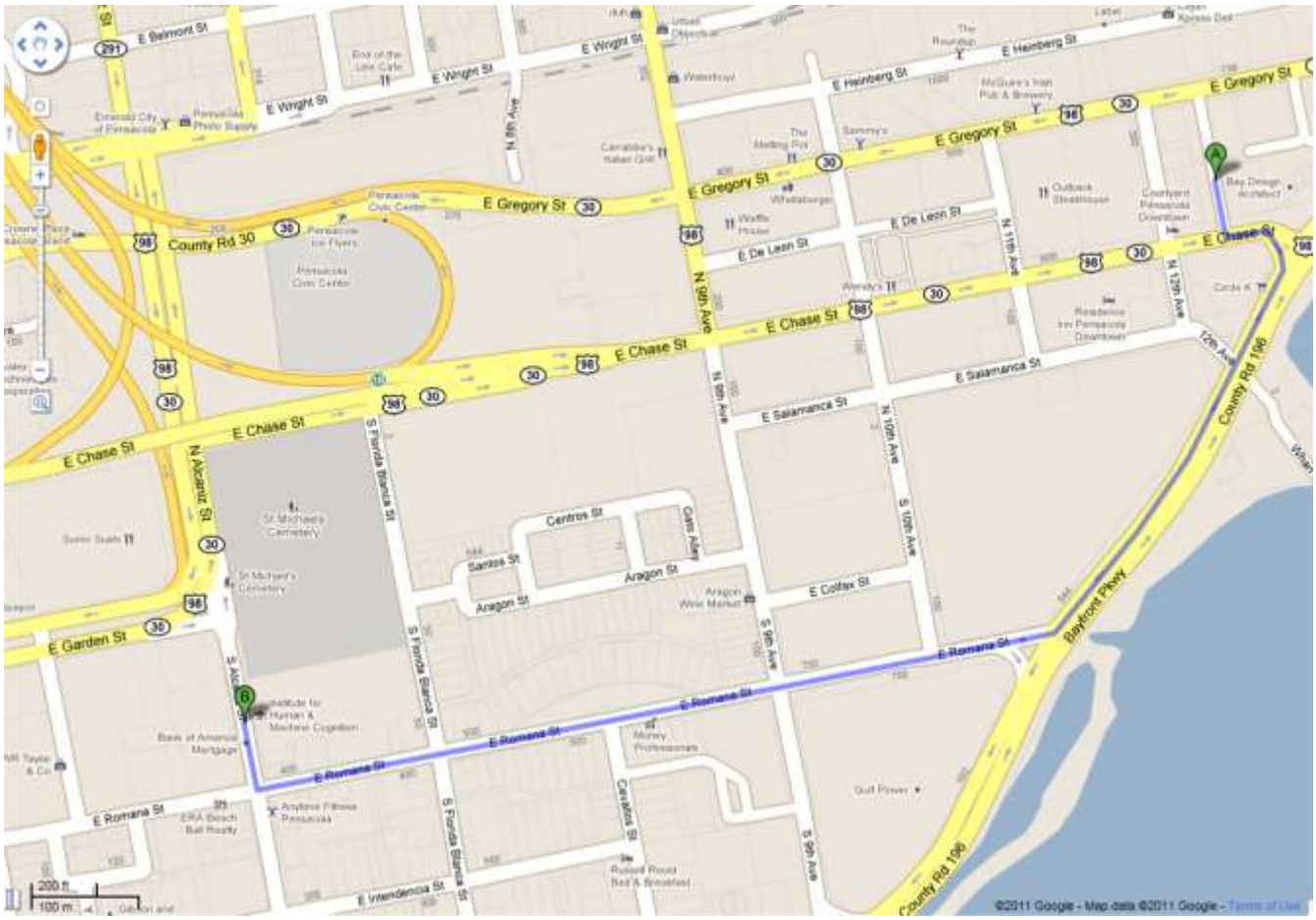


Walking from Courtyard Pensacola Downtown to IHMC

FROM: Courtyard Pensacola Downtown
700 E Chase Street
Pensacola, FL 32502
GPS: N 30.41687 W 87.20051

1. Head south toward E Chase St	177 ft
2. Turn left at E Chase St	121 ft
3. Turn right at Bayfront Pkwy/Country Rd 196	0.3 mi
4. Slight right at E Romana St	0.5 mi
5. Turn right at S Alcaniz St	210 ft
6. Destination on right	

TO: Florida Institute for Human & Machine Cognition
40 South Alcaniz Street
Pensacola, FL 32502
GPS: N 30.41284 W 87.20985

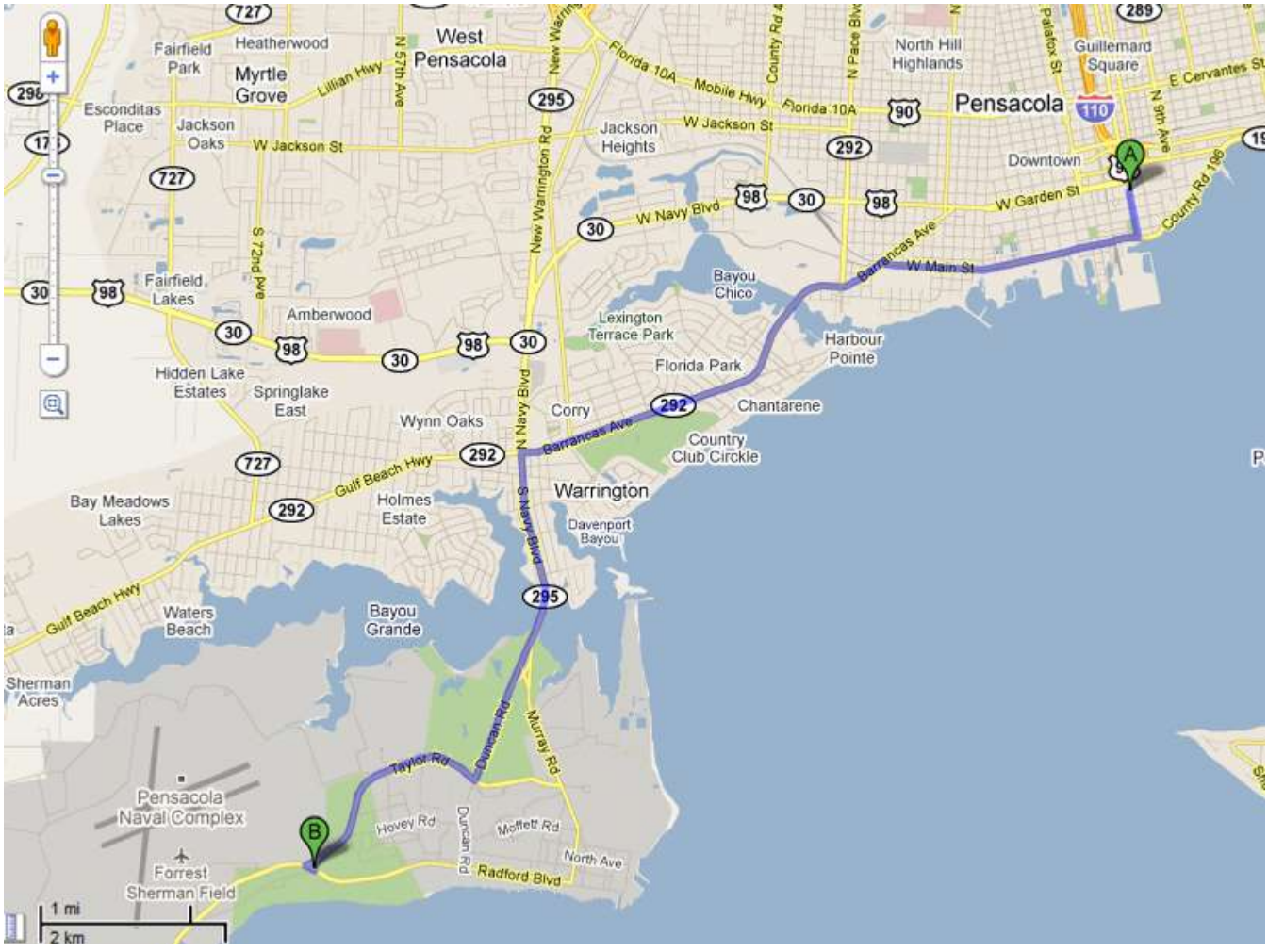


The **National Naval Aviation Museum** is located aboard Naval Air Station Pensacola, approximately seven miles west of downtown Pensacola. Parking and admission to the Museum are free.

FROM: Florida Institute for Human & Machine Cognition
40 South Alcaniz Street
Pensacola, FL 32502
GPS: N 30.41284 W 87.20985

1. Head south on S Alcaniz St toward E Romana St	0.3 mi
2. Turn right at County Rd 196/E Main St (continue to follow E Main St)	1.7 mi
3. Turn left at Barrancas Ave	2.9 mi
4. Turn left at S Navy Blvd	1.0 mi
5. Continue onto Duncan Rd	0.5 mi
6. Keep right at the fork (continue to follow Duncan Rd)	0.9 mi
7. Turn right at Taylor Rd	1.5 mi
8. Arrive at Radford Blvd	381 ft

TO: National Naval Aviation Museum
1750 Radford Blvd.
Pensacola, FL 32508
GPS: N 30.34787 W 87.30162



FROM: Florida Institute for Human & Machine Cognition
40 South Alcaniz Street
Pensacola, FL 32502
GPS: N 30.41284 W 87.20985

1. Head south on S Alcaniz St toward E Romana St	210 ft
2. Take the 1st left onto E Romana St	0.4 mi
3. Slight left at Bayfront Pkwy/County Rd 196 (continue to follow Bayfront Pkwy)	0.6 mi
4. Continue onto E Gregory St	0.3 mi
5. Continue onto FL-30 E/US-98 E/Pensacola Bay Bridge	4.5 mi
6. Take the exit toward Pensacola Beach/Fort Pickens	0.2 mi
7. Merge onto FL-399 S/Pensacola Beach Blvd (partial toll road)	1.3 mi
8. Destination will be on the left (U-turn may be necessary).	0.3 mi

TO: Grand Marlin Restaurant
400 Pensacola Beach Blvd.
Pensacola Beach, FL 32561
GPS: N 30.34380 W 87.15008