IP1

Effective Behavior of Random Media: An Error Analysis

Heterogeneous media, like a sediment, are often naturally described in statistical terms. How to extract their effective behavior on large scales, like the permeability in Darcy's law, from the statistical specifications? A practioneers numerical approach is to sample the medium according to these specifications and to determine the permeability in the Cartesian directions by imposing simple boundary conditions. What is the error made in terms of the size of this "representative volume element'? Our interest in what is called "stochastic homogenization' grew out of this error analysis. In the course of developing such an error analysis, connections with the regularity theory of elliptic equations and with concepts from statistical mechanics have emerged in a clearer way. We also gained an understanding of the structure of fluctuations of any solution: On large scales, the asymptotically Gaussian fluctuations are characterized by a single tensor-valued white noise. This characterization is "path-wise' and can also be extracted from the representative volume method. The latter is recent joint work with M. Duerinckx and A. Gloria.

Felix Otto
Max Planck Institute for Mathematics in the Sciences
Leipzig, Germany
Felix.Otto@mis.mpg.de

IP2

Stack em Up: Growth, Coarsening, and Alignment of Compositional Domains in Lipid Bilayer Membrane Systems

Multicomponent lipid bilayer membrane systems both natural and synthetic represent an interesting class of soft materials, which self-assemble in an aqueous environment and often display co-existing liquid-liquid or solid-liquid phases enriched in specific lipids. In this talk, I will discuss our recent progress in developing a quantitative understanding of the kinetics of compositional domain alignment and misalignment across opposing leaflets of planar lipid bilayers. I will also discuss the extension of this work to investigate the growth, coarsening, and alignment of compositional domains within planar membrane multilayer stacks.

Mikko Haataja
MAE Department
Princeton University
mhaataja@princeton.edu

IP3

Topology and Geometry of Dislocation Networks under Extreme Straining

Dislocations are ubiquitous in metals where their multiplication and motion presents the dominant mode of plastic response to straining. Under high-rate straining conditions, dislocation motion alone can become insufficient to relieve stress and to prevent other modes of inelastic response - twinning, phase transformations, cracking - from triggering. Here we report on a series of large scale atomistic and mesoscale simulations intended to probe the ultimate limits of dislocation-mediated crystal plasticity. The primary focus of our analysis is on topological and geometric characteristics of dislocation networks emerging during and post-straining. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Vasily Bulatov
Lawrence Livermore National Labs
bulatov1@llnl.gov

IP4

On the Trail of Hipsters and Robber Barons: Probing Microstructural Evolution Using Time-Resolved 3D X-Ray Imaging

Grain growth in polycrystalline materials is a war of attrition, culminating in the triumph of a few crystallites over all the rest. Mathematical analysis identifies two successful growth strategies: (1) relentlessly appropriating atoms at the fastest rate possible (the robber baron approach) or (2) feigning disinterest while profiting surreptitiously from the combat losses of belligerent neighbors (the hipster mentality). Employing time-resolved 3D imaging techniques, we have tested the predictive power of models for coarsening. X-ray microtomography was implemented to capture Ostwald ripening in semisolid Al-5 wt% Cu, and 3D x-ray diffraction microscopy (3DXRD) was used to study grain growth in Al-1 wt% Mg. The results represent not only a benchmark for validating computer simulations but also a foundation for establishing stochastic models for microstructural evolution.

Carl E. Krill III
Ulm University
carl.krill@uni-ulm.de

IP5

Theory and Challenges for Microstructure Evolution

We offer a view of microstructure evolution that is instrumental for our understanding of behavior of polycrystalline materials and for the design of future generation materials. A central problem is to develop technologies capable of producing an arrangement, or ordering, of the microstructure, in terms of geometry and crystallography, appropriate for a given application. New experimental techniques and especially developed large-scale simulations have led to the discovery of the grain boundary character distribution (GBCD), a statistic which details texture evolution. We explain the emergence of contemporary mass transport and entropy methods to develop the theory and, as a consequence, to identify the GBCD. Finally a glimpse of what to come.

David Kinderlehrer
Carnegie Mellon University
davidk@andrew.cmu.edu

IP6

Transforming Molecular Modelling with Applied Mathematics

In this talk I will describe our work over the past decade in pushing the boundaries of molecular simulation technology with the help of applied mathematics. Examples include using kernel methods from machine learning to improve sampling efficiency, systematic and controlled coarse graining both from quantum mechanical methods to interatomic potentials and from the latter to united atom models. Even well established ideas such as preconditioning have not fully penetrated the materials modelling field.

Most of these topics are linked by the notion of locality of interactions, a comprehensive mathematical treatment of which is still in the making.

Gábor Csányi
University of Cambridge
gc121@eng.cam.ac.uk

IP7
Title Not Available

Abstract not available at time of publication.

John Lowengrub
Department of Mathematics
University of California at Irvine
lowengrb@math.uci.edu

IP8
A Study of Speed Dependent Contact Angle Hysteresis

We study the interface dynamics and contact angle hysteresis in a two dimensional, chemically patterned channel described by the Cahn-Hilliard equation with a relaxation boundary condition. A system for the dynamics of the contact angle and contact point is derived in the sharp interface limit. From the behaviour of the solution of the contact angle dynamic equation, we observe stick-slip motion and contact angle hysteresis. Our analysis reveals the mechanism for the asymmetric speed dependent contact angle hysteresis observed experimentally. We also develop an efficient volume-preserving threshold-dynamics method for the wetting dynamics. Numerical examples are presented to verify our analysis.

Xiaoping Wang
Hong Kong University of Science and Technology
mawang@ust.hk

IP9
Mathematical Crystallography and Virology: Group and Graph Theoretical Approaches for the Characterization of Viruses Structure

Viruses are remarkable examples of order at the nano-scale. Many viruses, including the common cold, package their genomes into protein containers that are organized according to icosahedral surface lattices. We present here group and graph theoretical approaches for the characterization of virus structure, and demonstrate that these techniques provide new insights into virus assembly and the structural capsid transitions important for infection. We also show that these mathematical approaches can be exploited for the construction of nanoparticles in vaccine design.

Reidun Twarock
Departments of Mathematics and Biology
University of York
rt507@york.ac.uk

IP10
Title Not Available

Abstract not available at time of publication.

Christof Schütte
Freie Universität Berlin, Germany
schuette@mi.fu-berlin.de

IP11
Issues in the Multiscale Modeling and Methods of Solids

I shall discuss certain critical issues in the multiscale modeling and multiscale methods in the simulation of crystalline solids. In particular, the consistency and stability problems incurred by the coarse-graining procedure, multiscale approximation, and model reduction will be addressed through two representative examples: quasicontinuum method and Cauchy-Born rule. Our discussion covers both perfect crystal and defects.

Pingbing Ming
LSEC and Institute of Computational Mathematics
Chinese Academy of Sciences
mpb@lsec.cc.ac.cn

IP12
The 3D Structural Geometry of Nanoporous Gold and its Influence on Mechanical Response

The mechanical properties of nanoporous gold, a bicontinuous network structure, are strongly dependent on the size of the gold ligaments, and thus can be exploited through targeted annealing in order to tailor the structures for specific applications. While classical scaling laws for cellular materials have been shown to be poor predictors of modulus and strength due in part to the lack of explicit lengths in the constitutive laws, we show that the structural geometry envisaged is a more critical issue. The use of FIB-based tomography applied to representative volumes provides the needed morphological and most importantly - topological description of this unique cellular material, while micromechanical testing allows its correlation to stress-strain response and, in turn, additional insight into the observed size effects.

Erica Lilleodden
Helmholtz-Zentrum Geesthacht, Germany
erica.lilleodden@gkss.de

Kaixiong Hu, Markus Ziehmer
Helmholtz-Zentrum Geesthacht
kaixiong.hu@hzg.de, markus.ziehmer@hzg.de

IP13
Title Not Available

Abstract not available at time of publication.

Kaushik Bhattacharya
Howell N. Tyson Sr. Professor of Mechanics
California Institute of Technology
bhatta@caltech.edu

MS1
Auxetics and Spectrahedra

In materials science, auxetic behavior entails lateral widening upon stretching. For periodic framework structures, we have recently introduced a purely geometric approach to auxetics, based on the evolution of the periodicity lattice. We discuss resulting connections with convex algebraic geometry and elaborate on the role of spectrahedra for de-

termination of auxetic capabilities in periodic frameworks.

Ciprian S. Borcea
Department of Mathematics
Rider University
borcea@rider.edu

Ileana Streinu
Department of Computer Science
Smith College
istreinu@smith.edu

MS1

Entanglement in 2-Periodic Coordination Networks

With the program ToposPro [V.A. Blatov, A.P. Shevchenko, D.M. Proserpio Cryst. Growth Des. 2014, 14, 3576] we introduce a rigorous method to describe and classify the topology of entanglements (via Hopf links) between periodic networks using Extended Ring Nets that map rings and catenation of them. The ERN is able to map all patterns observed in a thousand of 2-periodic coordination polymers, showing that 16 ERNs are able to explain 2/3 of the structures observed. See L. Carlucci et al. Chem. Rev. 2014, 114, 7557. Support russian grant 14.B25.31.0005

Davide M. Proserpio
Dipartimento di Chimica
Università Degli Studi de Milano
davide.proserpio@unimi.it

Eugeny Alexandrov, Vladislav Blatov
Samara State Aerospace University, Samara, Russia
aleksandrov_ev1@mail.ru, blatov@samsu.ru

MS1

Polyhedral Origami

Origami, the art of paper folding, has recently found applications in the design of "exotic" meta-materials. Classical origami works with a flat piece of "paper", and the design problem amounts to finding the "creases" that allow the paper to fold to a desired 3D shape. A landmark technique for origami design is Robert Lang's Universal Molecule algorithm. In this talk, I present a generalization of Lang's method to polyhedral surfaces and discuss a number of new problems and applications.

Ileana Streinu
Department of Computer Science
Smith College
istreinu@smith.edu

MS1

On Algebraic and Geometric Properties of Hyperbolic Tilings

In this talk, we discuss two dimensional hyperbolic tilings together with their fundamental cell properties, symmetry and color symmetry group structures. Properties of hyperbolic tilings that are monocoronal will also be shown, where the vertex stars of the tiling are congruent. By a vertex star we mean a figure consisting of a vertex and its incident tiles. An application of color symmetry theory in studying the associated hyperbolic crystallographic group of a given hyperbolic tiling will also be presented.

Ma. Louise N. de las Penas
Department of Mathematics
Ateneo de Manila University
mdelaspenas@ateneo.edu

MS2

The Smectic Order of Wrinkles

A thin elastic sheet lying on a soft substrate develops wrinkled patterns when subject to some geometric incompatibility or to external forcing. Thin sheet elasticity and substrate response equip such wrinkles with some preferred spacing and with resistance to wrinkle curvature. The resultant liquid crystalline smectic behavior of such systems is in the focus of this talk, in which we use this analogy to explain several phenomena observed in elastic wrinkles and make further predictions.

Hillel Aharoni
The Racah Institute of Physics
The Hebrew University of Jerusalem
haharoni@sas.upenn.edu

Eleni Katifori
University of Pennsylvania
katifori@sas.upenn.edu

Randall Kamien
Physics Dept
University of Pennsylvania
kamien@physics.upenn.edu

MS2

Programming Shape: Tapping Braille, Folding Origami, Printing Flowers

Thin sheets are easier to bend than stretch. This simple observation leads to the constrained freedom underlies the shape shifting abilities of sheets that can accommodate globally periodic wrinkles, localized defect-like creases, and a host of variations in between. But how can we design shape (for function) ? I will describe our attempts to solve this problem in a few different settings that include programmable Braille, origami tessellations for complex surfaces, and 4d phytomimetic printing strategies, using a combination of experimental, computational and theoretical approaches.

L Mahadevan
Harvard University
lm@seas.harvard.edu

MS2

Mechanical Response and Geometrical Constraints in Folded Sheets

Origami has emerged as a powerful framework for designing 3D structures from flat sheets. In this talk, I will discuss how the mechanical properties of an origami sheet emerge from the fold pattern. I will show how the effective mechanical response is determined by the mechanical response of a single vertex and the network of folds joining them. The mechanics of a folded sheet shows a number of striking differences from the continuum mechanics of thin structures, including multi-stability, sensitivity to fold patterns and

hysteresis.

Christian Santangelo
UMass Amherst
csantang@physics.umass.edu

MS2

Symmetry Breaking in Indented Elastic Cones

Motivated by simulations of carbon nanocones (see Jordan and Crespi, Phys. Rev. Lett., 2004), we consider the minimum energy scaling law of an indented elastic cone in the Foppl-von Karman model. Assuming radial symmetry, we prove that there are three energetic regimes, depending on the indentation depth and the thickness. In the large indentation regime, we prove that the global energy minimizer is not radially symmetric by giving an explicit construction involving minimal ridges.

Sergio Conti
Institut fur Angewandte Mathematik
Universitat Bonn
sergio.conti@uni-bonn.de

Heiner Olbermann
Hausdorff Center for Mathematics & Institute for Appl. Math.
University of Bonn
heiner.olbermann@hcm.uni-bonn.de

Ian Tobasco
Courant Institute of Mathematical Sciences
New York University
tobasco@cims.nyu.edu

MS3

Atomistic Simulations of Line Defects at Interfaces

The motion of solid-solid and solid-liquid interfaces is often mediated by the formation and propagation of line defects (e.g., steps and disconnections). Kinetic theories for interface motion thus often require knowledge of the excess free energies of these line defects and their dependence on temperature. Unfortunately, such information is often difficult to extract directly from experimental measurements. In this work we describe two methods for computing excess free energies of line defects, based on (i) a combination of thermodynamic integration and non-equilibrium molecular dynamics "switching" techniques, and (ii) an extension of the capillary fluctuation method employed in previous studies of interfacial free energies. We demonstrate both approaches in equilibrium atomistic simulations of steps on (111) surfaces of elemental copper. We analyze the origins of the temperature dependence of the step free energy based on excess quantities formulated in a generalized Gibbs-Duhem analysis, and we show that methods (i) and (ii) yield consistent results if the system-size contributions to the step free energy arising from capillary fluctuations are accounted for.

Mark Asta, Rodrigo Freitas, Tim Frolov
University of California, Berkeley
mdasta@berkeley.edu, rodrigof@berkeley.edu, timfrol@berkeley.edu

MS3

Grain Growth in Alloys: Atomistic and Phase Field Perspectives

The evolution of the grain microstructure is a central issue in materials science. There is substantial current interest in the stabilization of nanocrystalline grain structures to maintain the enhanced properties of nanocrystalline metals as well as the influence of alloying on grain growth in conventional scale materials. It is known that alloying can have a profound influence on microstructure evolution. However, there is ambiguity about the relative roles of various mechanisms including thermodynamic stabilization due to alloy segregation, impurity drag and precipitate-boundary interactions. In this talk, we will use a combination of atomistic simulations and phase field modeling to elucidate the relative importance of these various mechanisms. Atomistic simulations will be used to investigate the thermodynamics of alloy segregation to grain boundaries, the influence of segregated species on grain boundary mobility and the variability of these factors with boundary type. Phase Field simulations will be used to study the influence of these factors, both individually and in concert, on the overall microstructure evolution.

S. M. Foiles, Fadi Abdeljawad, Christopher OBrien
Sandia National Laboratories
foiles@sandia.gov, fabdelj@sandia.gov, cjobrie@sandia.gov

MS3

Novel Application of Potts Model for Grain Growth During Welding using SPPARKS

Session code: AN; oral; No, transfer to poster The model presented in this paper simulates grain growth during welding in the vicinity of the weld. The model simulates the effects of velocity and shape of molten weld pool, and geometry and shape of heat affected zone (HAZ) on the resulting grain structure by melting the region within the molten pool and varying grain boundary mobility M based upon geometric proximity (alias for local temperature) to the weld pool. The model is implemented in the SPPARKS framework for kinetic Potts Monte Carlo simulations and qualitatively predicts trends in spatial and temporal microstructures relevant to real weld processes.

John A. Mitchell, Veena Tikare
Sandia National Laboratories
jamitch@sandia.gov, vtikare@sandia.gov

MS3

Dislocations, Trijunctions and Grain Boundary Motion

The effects of the atomic-scale structure of grain boundaries on grain growth are examined using phase field crystal calculations. We find that grains can translate during grain growth due to the climb, glide, and interactions of the dislocations that comprise the grain boundary and dislocation interactions at trijunctions. The effect of temperature and vacancy concentration on grain boundary structure, migration, and pinning will also be discussed.

Kevin McReynolds
Dept. of Materials Science and Engineering
Northwestern University
kevinmcreynolds2016@u.northwestern.edu

Peter Voorhees
Northwestern University
Dept. of Material Science and Engineering

p-voorhees@northwestern.edu

MS4

Mathematical Modeling of Multilayer 2D Materials

The design of multilayer 2D materials with specific electronic, optical, and mechanical properties is a hot topic in physics and materials science. In this talk, I will first recall the remarkable electronic properties of monolayer 2D materials, such as graphene sheets. I will then present tight-binding and DFT models allowing one to understand, or even predict, the electronic properties of monolayer 2D materials, as well as the ones of composite 2D materials consisting of stacks of monolayers of different materials. Although some progress has recently been made in the field, many problems remain essentially open. The main difficulty is to take into account the non-periodicity generated by both the incommensurabilities of the periods of the different monolayers, and the presence of defects. The results I will present have been obtained in the framework of a collaboration with the groups of Mitch Luskin (mathematics, University of Minnesota) and Tim Kaxiras (physics, Harvard).

Eric Cances
Ecole des Ponts and INRIA, France
cances@cermics.enpc.fr

MS4

Fast Algorithms for Localization of Kohn-Sham Orbitals

Given a set of Kohn-Sham orbitals from an insulating system, it is often desirable to build a set of localized basis functions for the associated subspace. In this talk we present a simple, robust, and parallelizable algorithm to construct a set of (optionally orthogonal) localized basis functions known as the selected columns of the density matrix (SCDM). In addition, we will discuss ways to accelerate the basic SCDM algorithm and make it even more computationally efficient.

Anil Damle
Stanford University
damle@stanford.edu

MS4

A QM/MM Model for Material Interfaces

Material interfaces are responsible to a wide variety of material properties. However, existing results from electronic structure calculations are often limited to cases with supercells, flat geometry, and periodic boundary conditions. We present a QM/MM coupling method, where the huge number of degrees of freedom are reduced by using a boundary element type of method. This allows us to eliminate the influence from periodic images, and incorporate the geometry of the interfaces into consideration.

Xiantao Li
Department of Mathematics
Pennsylvania State University
xli@math.psu.edu

MS4

Computing the Response Functions of Disordered Solids

Periodicity of crystal structures can be broken by a magnetic field or disorder. The latter may be due to either thermal motion of the nuclei or by the imperfections introduced during the fabrication. The effects cannot be neglected since they determine the low-temperature behavior of the response functions. In this talk I will present an efficient, stable and accurate method based on operator algebras for computing correlation and response functions of aperiodic homogeneous systems. It consists of controlled finite-volume approximations which converge exponentially fast to the thermodynamic limit. Rigorous convergence estimates and numerical applications will be presented. The latter include computations of the transport coefficients of integer quantum Hall systems and topological insulators, as well as of the electric polarization and magneto-electric response function.

Emil Prodan
Yeshiva University, New York
prodan@yu.edu

MS5

The Spectrum of Composite Media in Two Dimensions and Energy Harvesting

There is much current interest in energy harvesting, one aspect of which is to construct optical systems capable of absorbing solar energy over a broad range of wavelengths. One way of doing this for which there are a number of striking theoretical and experimental results is to do this using appropriately structured thin films composed of metal and dielectric components. I will review established and recent results in this field, linking experimental results on broadband absorbers with the requirements on the spectrum of the metal/dielectric composite material. The importance of branch cuts or quasi branch cuts in the spectrum will be emphasised. together with the role of the strong dispersion given by the metallic component of the structure.

Ross McPhedran
Professor of Physics,
Department of Physics, The University of Sydney
ross@physics.usyd.edu.au

MS5

Bounds on the Transient Response of Composites and Bodies

Bounds on the complex dielectric constant of a two-component material at fixed frequency were derived about 35 years ago independently by Milton and Bergman using the analytic representation formula for the effective dielectric constant as a function of the component dielectric constants. These bounds were subsequently generalized to elasticity in works of Berryman, Gibiansky, Lakes and Milton, using the variational principles of Cherkaev and Gibiansky. All these bounds are applicable when the applied fields are time harmonic. But what happens when the applied fields are not time harmonic? One would like to bound for each moment in time, the transient response of a composite. We will show how these can be obtained using integral representation formulas for the response. This approach is applicable, not just to the transient response of composites but also to the transient response of two-phase bodies, and can be used in an inverse way to determine information about the interior geometry. This is joint work

with Ornella Mattei.

Graeme Milton
Distinguished Professor of Mathematics
Department of Mathematics University of Utah
milton@math.utah.edu

Ornella Mattei
University of Brescia
ornella.mattei@ing.unibs.it

MS5

Generalized Wannier Functions

For Schrodinger operators with a gap in the energy spectrum, we construct a complete, orthonormal basis function set for the invariant space corresponding to the spectrum below the spectral gap, which are exponentially localized around a set of closed surfaces of monotonically increasing sizes. Complex scaling technique and theory of complex symmetric operators are employed to determine sharp estimates on the exponential decay rate of the functions. Since there is a large degree of freedom in choosing the shape of the closed surfaces, the Wannier functions so constructed can be useful in the analysis of various defects in homogeneous materials.

Emil Prodan
Yeshiva University, New York
prodan@yu.edu

MS6

Algorithms for Weighted (Anisotropic) Mean Curvature Motion of Networks

I will describe recent progress in extending Merriman, Bence, and Osher's threshold dynamics (MBO) algorithm for mean curvature motion (which in its original form works only for networks with isotropic and equal suface tensions) to grain boundary networks where the surface energy of each interface can potentially have a different anisotropic (normal dependent) energy density.

Selim Esedoglu
University of Michigan
esedoglu@umich.edu

MS6

Density Functional Perturbation Theory for Large Systems

Phonons and related properties are important in a number of fields in physics, chemistry and materials science. Phonon calculations require the dynamical matrix, which is related to the second order derivatives of the ground state total energy with respect to the atomic position, and the phonon frequencies are the eigenvalues of the dynamical matrix. In Kohn-Sham density functional theories, the most straightforward way for computing the dynamical matrix is the frozen phonon approach, which perturbs each atom towards each of the three dimensional directions in real space. Hence even lowest order finite difference approximation requires 3N+1 ground state calculations where N is the number of atoms. This procedure is prohibitively expensive and the cost scales as $O(N^4)$. The complexity is the same when density functional perturbation theory (DFPT) is used, due to a large number of linear to be solved. We develop an efficient numerical method to compress the linearly dependent equations, which allows phonon calculations to be performed via density functional perturbation theory with reduced complexity.

Lin Lin
University of California, Berkeley
Lawrence Berkeley National Laboratory
linlin@math.berkeley.edu

Ze Xu
University of California, Berkeley
number1.xuze@berkeley.edu

Lexing Ying
Stanford University
Department of Mathematics
lexing@stanford.edu

MS6

Solitary Waves in Two Dimensional Lattices

Abstract not available

Liping Liu
Department of Math, Mechanical Engineering
Rutgers University
liu.liping@rutgers.edu

MS6

The String Method for Saddle Points Search

The dynamics of complex systems is often driven by rare but important events. Well known examples include nucleation events during phase transitions, conformational changes in macromolecules, and dislocation dynamics in crystalline solids. The main object of interest in these problems is the saddle points of the potential or free energy of the system. These saddle points act as bottlenecks (transition states) for the barrier-crossing event. In this talk, we show how the string method, which was originally developed to compute minimum energy paths between two given states, can be used to compute saddle points for a given minimum of the potential or free energy.

Weiqing Ren
National University of Singapore and IHPC, A-Star
matrw@nus.edu.sg

MS7

Critical Scaling with Strain Rate in Overdamped Sheared Disordered Solids

In the limit of quasistatic shear, disordered solids demonstrate non-equilibrium critical behavior including power-law distributions of avalanches. Using molecular dynamics simulations of 2D and 3D overdamped binary LJ glasses, we explore the critical behavior in the limit of finite strain rate. We find a system size dependent threshold strain rate for avalanches and use finite-size scaling to find the critical exponents characterizing shear stress, kinetic energy, and measures of temporal and spatial correlations.

Joel T. Clemmer, Mark Robbins
Johns Hopkins University

jclemme3@jhu.edu, mr@jhu.edu

MS7

Direct Measurements of Transformation Barriers in Glasses

In a model atomic glass, a good correlation is established between the low shear stress thresholds measured locally and the plastic rearrangements observed during a mesoscopic loading. This local yield stress field shows an overall better prediction power of the plastic activity location in comparison with more conventional structural properties. Most importantly, the incipient transitions thus detected are shown to be persistent with the plastic deformation, even after many plastic rearrangements.

Sylvain Patinet, Damien Vandembroucq
Laboratoire PMMH, ESPCI
sylvain.patinet@espci.fr, damien.vdb@gmail.com

Michael L. Falk
Materials Science and Engineering
Johns Hopkins University
mfalk@jhu.edu

MS7

Softness: A Structural Approach to Failure or Relaxation in Disordered Systems

All solids flow at high enough applied stress and melt at high enough temperature. Crystalline solids flow and premelt via localized particle rearrangements that occur preferentially at structural defects known as dislocations. The population of dislocations therefore controls both how crystalline solids flow and how they melt. In disordered solids, there is considerable evidence that localized particle rearrangements induced by stress or temperature occur at localized flow defects but all attempts to identify them directly from the structure have failed. Here we introduce a novel application of machine learning data mining methods to diagnose flow defects, or soft particles from their local structural environments. We follow the softness of each particle as it evolves under deformation or temperature. Our results show that machine learning methods can be used to gain a conceptual understanding that has not been achieved with conventional approaches.

Andrea Liu
Physics and Astronomy
University of Pennsylvania
ajliu@seas.upenn.edu

MS7

Strain Localization and Fracture in Metallic Glass

Metallic glasses are a new type of alloy whose atoms form an amorphous structure in contrast to most metals. They have many favorable properties, but can break in some circumstances depending on their method of preparation. This talk will develop an Eulerian quasi-static projection method for simulating a physical model of a metallic glass based on the shear transformation zone theory. The simulations can be used to predict strain localization and fracture in these materials.

Chris H. Rycroft
Harvard University
chr@seas.harvard.edu

MS8

Transient Shear Banding and the Two-Fluid Rolie-Poly Model

In this talk we delve into the transient characteristics of shear banded flow of polymer solution. We focus on how stress-concentration coupling affects transients under shear flow. We will focus on 4 time scales: i. Onset of transient banding, ii. Onset of local concentration gradients, iii. Onset of large concentration differences, iv. Long-time diffusive process to steady state. Ultimately, we show that the model captures several transient phenomena on experimental time scales with realistic parameters.

Michael Cromer
University of California, Santa Barbara
mec2sma@rit.edu

MS8

Shear Banding in Entangled Polymeric Fluids and the Origin and Role of Spatially Inhomogeneous Dynamics

Entangled polymers and wormlike micelles have strong non-linear rheology, which arises because of the entanglements present in these fluids. In some cases the rheology has a multivalued flow curve, in which there are two stable shear rates for a range of shear stresses. This can give rise to *shear banding*, in which the fluid partitions into a superposition of two viscosities at a given stress. This raises the problem of *stress selection*: how to choose at which stress such a fluid can transit between the states of different microstructure. A unique stress can be selected, as found in experiments, by enlarging the constitutive equations to include non-local contributions to the dynamics, typically in the form of spatial derivatives. This talk will describe shear banding phenomena recently inferred in entangled polymers, and discuss different physical mechanisms for the spatial gradient terms and their manifestations in models for entangled polymeric fluids.

Elian Masnada, Peter Olmsted
Georgetown University
elian.masnada@gmail.com, peter.olmsted@georgetown.edu

MS8

Writhe and Mutual Entanglement Combine to Give the Entanglement Length

Session code: AB; oral; Yes, transfer to poster We propose a new method to estimate N_e, the entanglement length, that incorporates both local and global topological characteristics of chains in a melt under equilibrium conditions. This estimate uses the writhe of the chains, the writhe of the primitive paths and the number of kinks in the chains in a melt. An advantage of this new method is that it works for both linear and ring chains, works under all periodic boundary conditions, does not require knowing the contour length of the primitive paths and it does not rely on a smooth set of data. We apply this method to linear finitely extendable non-linear elastic chains and we observe that our estimates are consistent with those from other studies.

Eleni Panagiotou
University of California Santa Barbara

lnpanagiotou@yahoo.com

Martin Kroeger
ETH Zurich
mk@math.ethz.ch

Kenneth Millett
University of California Santa Barbara
millett@math.ucsb.edu

MS8

Modeling Thixotropic Yield Stress Fluids As a Singular Limit of Viscoelasticity

Many yield stress fluids exhibit behaviors which cannot be described by simple yield stress models, such as yield stress hysteresis, delayed yielding and thixotropy. The talk will review efforts to model such behaviors as a singular limit of viscoelasticity, in which a relaxation time becomes large. This naturally leads to a small parameter and analysis by the methods of singular perturbation and matched asymptotics. The dynamics of yielding and unyielding, oscillatory shear flows, and formation of shear bands will be discussed.

Michael Renardy
Department of Math, Virginia Tech
mrenardy@math.vt.edu

Taige Wang
Department of Math., Virginia Tech
tigerwtg@math.vt.edu

MS9

Shape-Based Modeling of the Self-Assembly Processes

Shape is an important mediator of self-assembly on the micro- and nanoscale and crucial for physical properties and function. Here, we discuss the modeling of anisotropic nanocrystals with and without interactions. Using particle-based computer simulations, we demonstrate how shape alone can control the geometry of superlattices, propensity and efficiency of the self-assembly process, and how to design shapes for targeted behavior. Driving shapes out of equilibrium introduces dynamic phenomena not achievable otherwise.

Michael Engel
Deparment of Chemical Enginering
University of Michigan
engelmm@umich.edu

MS9

Coarse-Grained Mesoscale Modeling for Deposition-Diffusion and Reaction-Diffusion Systems

The 2012 DOE BESAC Mesoscale Report identified mesoscale systems as providing new opportunities for development of functional materials and optimizing energy-relevant processes. A challenge is to develop effective conceptual and modeling formulations between the discrete atomistic and macroscopic continuum levels. I discuss two examples: coarse-grained treatments of assembly or growth of unstable films during deposition, and generalized hydrodynamic treatments of catalysis in mesoporous materials. Both require suitable description of mesoscale transport and fluctuations.

James Evans
Ames LaboratoryUSDOE
Dep of Physics & Astro and Dep of Math, Iowa State Univ
evans@ameslab.gov

Tiago de Oliveira
Iowa State University
Universidade Federal de Vicosa
tiago@ufv.br

Yong Han
IOwa State University
yhan.ameslab@gmail.com

Da-Jiang Liu, Andres Garcia
Iowa State University
dajiang@fi.ameslab.gov, andresg@iastate.edu

MS9

Multiscale Modeling of Nanocrystal Growth in Solution

Achieving controlled, shape-selective syntheses of colloidal nanomaterials is an important goal. A deep, fundamental understanding of the phenomena that promote selective growth is important to this end. I will discuss our efforts to understand the workings of PVP, a structure-directing molecule that facilitates the formation of 100 Ag nanoparticles. In these studies, we use first-principles density-functional theory, molecular dynamics simulations, and continuum theory to predict PVP-induced Ag nanocrystal shapes in the 10-100 nm size range.

Kristen Fichthorn
Penn State University
fichthorn@psu.edu

MS9

Stratification of Markov Processes for Rare Event Simulation

Ensemble sampling schemes decompose target averages into easier subproblems that can be solved in parallel. The most basic version computes averages with respect to a given density, a generalization of Umbrella Sampling for free energies. We develop a careful understanding of the accuracy of the scheme, sufficiently detailed to explain the success of umbrella sampling and to suggest improvements including adaptivity. For equilibrium versions, we developed error bounds revealing that the existing understanding is incomplete.

Jonathan Weare
University of Chicago
Department of Statistics and the James Franck Institute
weare@uchicago.edu

MS10

Discovery of Metastable and Transition States Using the Concurrent Adaptive Sampling Method

Many existing sampling methods can efficiently obtain conformations of bio-molecules, but they often destroy real kinetics. Hence, a new sampling method, called Concurrent Adaptive Sampling, has been developed to efficiently ob-

tain thermodynamic and kinetic properties. The method adaptively creates macrostates and explores the free energy landscape, which can be in arbitrary dimensions, by running a large number of short trajectories at equilibrium. Here, we present the new methodology and results from penta-alanine and triazine polymers.

Surl-Hee Ahn
Stanford University
sahn1@stanford.edu

Eric F. Darve
Stanford University
Mechanical Engineering Department
darve@stanford.edu

MS10

Bayesian Inference Using Gaussian Process Metamodel in Biomechanical Imaging

Modeling of biomechanical imaging is hindered by uncertainties. In the case of soft tissue parametric studies, calibrating the soft tissue posterior parameters in a Bayesian framework that employs Markov Chain Monte Carlo methods elevates this limitation. Our methodology facilitates the development of a Gaussian process model and performs a Bayesian inference, thus providing a solution to the challenge of finding the right model for the analysis.

Assimina A. Pelegri, Colin Cui
Rutgers - The State University of New Jersey
pelegri@jove.rutgers.edu, colstat@gmail.com

Xiaodong Zhao
J P Morgan
zhaoxd.sn@gmail.com

MS10

Data-Driven Parameterization of Memory Kernel in the Generalized Langevin Equation

We propose a method based on appropriate parameterization to compute the memory kernel of the generalized Langevin Equation (GLE). The proposed method is data-driven as kernel is constructed by merely using trajectory data. While the first-order approximation is consistent with the Makovian approximation, higher order approximations can be systematically derived. The approximated kernel formulation satisfies the second fluctuation-dissipation conditions naturally and enables us to eliminate the history-dependence by introducing auxiliary variables of Markovian process.

Huan Lei, Nathan Baker
Pacific Northwest National Laboratory
huan.lei@pnnl.gov, nathan.baker@pnnl.gov

Xiantao Li
Department of Mathematics
Pennsylvania State University
xli@math.psu.edu

MS10

Efficient Failure Probability Calculation Through Mesh Refinement

We present a novel way of accelerating hybrid surrogate methods for the calculation of failure probabilities. The main idea is to use mesh refinement in order to obtain improved local surrogates of low computation cost to simulate on. These improved surrogates can reduce significantly the required number of evaluations of the exact model (which is the usual bottleneck of failure probability calculations). Meanwhile the effort on evaluations of surrogates is dramatically reduced by utilizing low order local surrogates.

Jing Li
Pacific Northwest National Lab
jing.li@pnnl.gov

Panos Stinis
Northwest Institute for Advanced Computing
University of Washington
panagiotis.stinis@pnnl.gov

MS11

Stochastic Homogenization and the Random Conductance Model

I will review some of my contributions to homogenization theory of the Random Conductance Model. This includes the following topics:

1. A quenched invariance principle (i.e., scaling to Brownian motion for a.e. sample of the environment) of the random walk among non-elliptic random conductances,
2. Anomalous heat-kernel decay due to trapping in i.i.d. conductance environments with heavy tails at zero,
3. Existence of multiple zero-tilt Gibbs states and a Gaussian Free Field limit of the fluctuations for a class of gradient fields with non-convex interactions,
4. A Gaussian limit theorem for the effective conductivity under linear boundary conditions.

My talk will be mostly an overview with particular emphasis on those aspects that I deem to be interesting for the audience of the conference.

Marek Biskup
UCLA
Department of Mathematics
biskup@math.ucla.edu

MS11

Eigenvalue Fluctuations for Lattice Anderson Hamiltonians

We will discuss a homogenization problem for the eigenvalues of the so-called Anderson Hamiltonian. This type of problem was studied by Guillaume Bal, based on the functional analytic method, where the convergence of eigenvalues and a Gaussian fluctuation were proved for the space dimensions $d \leq 3$. We propose a probabilistic approach which yields a similar conclusion in general dimensions. Key tools are the concentration of measures and a martingale central limit theorem.

Ryoki Fukushima
Research Institute for Mathematical Sciences
Kyoto University, Japan
ryoki@kurims.kyoto-u.ac.jp

Marek Biskup
UCLA
Department of Mathematics
biskup@math.ucla.edu

Wolfgang Koenig
Weierstrass Institute for Applied Analysis and Stochastics
koenig@wias-berlin.de

MS11

A Quantitative Two-Scale Expansion in Stochastic Homogenization

We study linear elliptic systems with rapidly oscillating, random (stationary and ergodic) coefficients. We consider the classical two-scale expansion for such systems and establish an H^1-error estimate. While estimates on the error of the two-scale expansion are well understood in the case of (deterministic) periodic homogenization, the situation for random coefficients is more subtle and it turns out that the error is highly sensitive to the mixing properties and the strength of correlations of the random coefficients.

Stefan Neukamm
Technische Universität Dresden
Institute for Scientific Computing
stefan.neukamm@tu-dresden.de

Felix Otto
Max Planck Institute for Mathematics in the Sciences
Leipzig, Germany
Felix.Otto@mis.mpg.de

Antoine Gloria
Université Libre de Bruxelles
Département de mathématique
agloria@ulb.ac.be

MS11

Homogenization of Quasiperiodic Constitutive Relations

We utilize the cut-and-projection method to homogenize quasiperiodic structures. The cut-and-projection operator defines quasiperiodic heterogeneous materials by cutting a higher dimensional periodic medium with a hyperplane and projecting it onto a lower dimensional spatial space. We use the extension of two-scale convergence to *two-scale-cut-projection convergence* presented in [Bouchitt, et. al., Multiscale Model. Simul. 8 (2010)] and we characterize the corresponding two-scale limits of differential operators. The method is demonstrated on an electrostatic example.

Niklas Wellander
Swedish Defence Research Agency, FOI
niklas.wellander@foi.se

Sébastien Guenneau
Institut Fresnel
sebastien.guenneau@fresnel.fr

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

MS12

The Statistical Mechanics of Singular Sphere Packings

What are all the ways to arrange N hard spheres to form a rigid cluster? The answer brings insight to a number of phenomena in materials science, from nucleation, to emergence, to self-assembly. We enumerate packings of $N \leq 19$ spheres using a deterministic numerical algorithm, whose completeness could be addressed using geometrical methods. We next ask: what is the free energy of the clusters when the spheres interact with a very short-range potential? For all so-called "regular' clusters, this can be evaluated using a harmonic approximation for the energy. However, the list contains a great many "singular' clusters, which correspond to singular solutions to a set of algebraic equations. These are also the clusters one sees with unusually high probability in experiments. We show how to compute the leading-order contribution to their free energy, and discuss implications for problems in materials science.

Miranda Holmes-Cerfon
Courant Institute of Mathematical Sciences
holmes@cims.nyu.edu

Yoav Kallus
Santa Fe Institute
yoav@santafe.edu

MS12

Algorithmic Self-Assembly and Self-Similar Structures

Recursive processes and self-similarity of form and function can be seen in many natural phenomena. Controlled algorithmic self-assembly, in particular DNA self-assembly has shown grand progress in recent years. Advances have been made to control the assembly process such that structural recursive growth with self-similar functionality of the components is becoming feasible. We describe a model, and experimental results supporting it, where the building blocks of the assembly process are capable of transmitting and receiving binding site activation signals thereby accomplishing assembly in stages. Within this model, it can be shown that a recursive assembly of archetypal self-similar aperiodic structures can be realized.

Natasha Jonoska
University of South Florida
Department of Mathematics
jonoska@usf.edu

MS12

What Role for Entropy in Stability and Growth of Quasicrystals?

How do crystals grow? This question is important for all crystals, but insights may be gained from studying quasicrystals. The emerging view is that clusters are important, especially clusters with portions of icosahedral symmetry. Entropy may be key to stabilizing such clusters. I will discuss experimental results (Tsai-type quasicrystals, Rappaz's findings on gold fining), simulation results (Glotzer's group), and new problems in discrete geometry.

Jean Taylor
New York University
CIMS

jtaylor@cims.nyu.edu

MS12

Clusters of Polyhedra in Spherical Confinement

Minisymposium Session Code: O Packing objects of a given shape as densely as possible within a confining geometry is an intriguing puzzle with applications ranging from colloidal crystallization to industrial packaging. Despite their widespread relevance, however, solutions to packing in confinement problems remain largely unexplored. We present simulation results for dense packings of the Platonic solids in spherical confinement, for up to $N = 60$ constituent particles, and discuss the role of confinement in resultant diverse cluster structures.

Erin G. Teich
University of Michigan
Applied Physics Program
erteich@umich.edu

Greg Van Anders
University of Michigan
grva@umich.edu

Daphne Klotsa
University of Michigan
Current affiliation: University of North Carolina
dklotsa@email.unc.edu

Julia Dshemuchadse
University of Michigan
djulia@umich.edu

Sharon C. Glotzer
Chemical Engineering
University of Michigan
sglotzer@umich.edu

MS13

Regularizing Rigidifying Curves to Understand the Low-Energy Deformations of Thin Shells

It is much harder to stretch a piece of paper than bend it. We exploit this fact to simplify the elastic energy of a thin shell. We accomplish this by extending the linear isometric displacements, displacements that do not cause stretching to lowest order, to low energy Nambu-Goldstone modes. This approach fails in an interesting way in the vicinity of rigidifying curves, curves with zero normal curvature, because half of the linear isometries are divergent there. We regularize these divergences by including the nonlinearities in strain. We explore the relationship between these modes and folding along curves of zero normal curvature.

Salem H. Al Mosleh
University of Massachusetts, Amherst
salmosle@physics.umass.edu

Christian Santangelo
UMass Amherst
csantang@physics.umass.edu

MS13

Non-Developable Isometries in Elastic Sheets

Imposing a curved, non-develpable shape on a naturally-flat sheet, generates in it strain and consequently elastic stress. This familiar motif is a consequence of Gauss theorema Egregium, which posits that there exists no isometric map between two surfaces of different Gaussian curvatures. However, recent experimental and theoretical work reveals that imposing curvature on elastic sheets often leads to non-developable shapes (riddled with wrinkles or other kinds of micro-structues) with arbitrarily small strain. In this talk I will provide a theoretical framework to this class of "asymptotic isometries" and the morphological transformations associated with transitions between developable and non-developable isometries.

Benny Davidovitch
University of Massachusetts Amherst
Physics Department
bdavidov@physics.umass.edu

MS13

Wrinkling Reveals New Isometries of Elastic Sheets and Shells

Thin elastic objects are difficult to stretch rather than bend and so their isometries are a natural way of understanding their deformation. I will discuss two problems arising from the indentation (poking) of elastic objects in which the classic isometries are not observed. Instead, the object wrinkles and in so doing reveals a new isometry of the object in question.

Dominic Vella, Matteo Taffetani
Mathematical Institute
University of Oxford
dominic.vella@maths.ox.ac.uk,
matteo.taffetani@maths.ox.ac.uk

Benny Davidovitch
University of Massachusetts Amherst
Physics Department
bdavidov@physics.umass.edu

MS13

Geometric Defects in Thin Elastic Structures

I will discuss recent developments in analytic, geometric and numerical techniques for studying hyperbolic free sheets, i.e thin elastic objects, with an intrinsic non-Euclidean (hyperbolic) geometry. Among these developments are (i) advances in Discrete differential geometry of hyperbolic surfaces; (ii) regularity, rigidity and flexibility for solutions of hyperbolic Monge-Ampere equations; and (iii) the role, in soft matter, of "geometric" defects that do not concentrate energy. I will also discuss the physical implications of these results.

Shankar C. Venkataramani
University of Arizona
Department of Mathematics
shankar@math.arizona.edu

Toby Shearman
Program in Applied Mathematics
University of Arizona
tsherman@math.arizona.edu

John A. Gemmer
Brown University

john_gemmer@brown.edu

MS14

Recent Advances in the Simulation of Grain Boundary Migration and Related Phenomena: From the Atomistic to the Mesoscopic Scale

We combined atomistic simulation and experimentation in bicrystals to study the migration behaviour and energy anisotropy of various tilt, twist and mixed grain boundaries. The results of these investigations were utilized in mesoscopic models for grain growth to understand the interplay of different types of grain boundaries undergoing grain growth. Data analytics techniques were applied to extract long-range dependencies on crystallography that are not evident from simpler analysis.

Luis Barrales-Mora, Dmitri A. Molodov
RWTH Aachen University
barrales@imm.rwth-aachen.de,
molodov@imm.rwth-aachen.de

Markus Kühbach
Institute of Physical Metallurgy and Metal Physics
RWTH Aach
kuehbach@imm.rwth-aachen.de

Christian Mieen
Institute of Physical Metallurgy and Metal Physics
RWTH Aachen University
miessen@imm.rwth-aachen.de

MS14

Recent Advances in the Full Field Modeling of Recrystallization and Grain Growth Using the Level Set Approach

Recently, an original full field model using the level set method in a finite element framework has been introduced in order to simulate in 2D or 3D large scale grain growth and recrystallization problems at the mesoscopic scale. This approach allows to deal with an important number of microstructure characteristics (dislocation density, second phase particles, high anisotropy of boundary energy...). Illustrations will concern SRX/DRX/GG of 304L stainless steel and SRX/GG of Inconel 718.

Marc Bernacki, Benjamin Scholtes
Mines ParisTech
marc.bernacki@mines-paristech.fr,
benjamin.scholtes@mines-paristech.fr

Nathalie Bozzolo
Mines ParisTech
Cemef
nathalie.bozzolo@mines-paristech.fr

MS14

Graph Kernel Approaches to the Transgranular Network

Polycrystalline materials can be modeled as networks of interconnected features, and their properties can be determined from network characteristics. For example, the minimum energy intergranular fracture surface is the min cut of the grain boundary (or intergranular) network. Likewise, the stress corrosion process proceeds along the penetration front of the same network. While intergranular network properties have been actively researched, less attention has been focused on the grain (or transgranular) network. The transgranular network influences material properties that depend on grain connectivity, such as load bearing, grain growth, and fracture initiation. In this study, we apply graph kernel analysis along with machine learning to elucidate the features of the transgranular network that are associated with rare events, such as abnormal grain growth or stress hot spot formation. We find that both phenomena depend on long-range network interactions, and we compare several non-local graph kernels in order to extract the network features that govern the events of interest.

Elizabeth Holm
Carnegie Mellon University
eahom@andrew.cmu.edu

Brian DeCost
Carnegie Mellon
bdecost@cmu.edu

Anika Mangel
Carnegie Mellon University
mangel@cmu.edu

MS14

Coupled Modeling of Deformation and Recrystallization of Texture in Uranium

Abstract not available

Marko Knezevic
University of New Hampshire
marko.knezevic@unh.edu

MS15

Chebyshev Filtered Subspace Iterations Within the Framework of Discontinuous Galerkin Density Functional Theory for Large Scale Abinitio Simulations

Discontinuous Galerkin Density Functional Theory (or DG-DFT) is a Density Functional Theory method based on the (interior penalty) Discontinuous Galerkin formalism. This approach employs Adaptive Local Basis functions (ALBs) generated on-the-fly to capture the local material physics and allows one to construct an efficient discretization of the Kohn-Sham Hamiltonian such that chemical accuracy can be attained using only few tens of degrees of freedom per atom. A pervasive issue however, is obtaining the electron density (and subsequently, ground state properties) from the discretized Hamiltonian in an efficient and scalable manner. We show in this work how Chebyshev Filtered Subspace iterations can be used to mitigate this issue and how it can help in pushing the envelope of large scale complex materials simulations with DG-DFT. In particular, this strategy makes it possible to attack complex materials science problems involving many thousands of atoms routinely. We describe how the subspace filtering steps can be done in an efficient and scalable manner using a two dimensional parallelization scheme. The on-the-fly nature of the ALBs requires additional care for carrying out the subspace iterations and we elaborate on this aspect. Scalability properties are discussed in detail. Performance comparisons with alternative techniques are presented. We will end with a discussion of outstanding issues and possible avenues for addressing these issues.

Amartya S. Banerjee, Wei Hu

Lawrence Berkeley National Laboratory
asb@lbl.gov, whu@lbl.gov

Lin Lin
University of California, Berkeley
Lawrence Berkeley National Laboratory
linlin@math.berkeley.edu

Chao Yang
Lawrence Berkeley National Lab
cyang@lbl.gov

John Pask
Lawrence Livemore National Lab
pask1@llnl.gov

MS15

Acceleration of Hybrid Density Functional Computations Using Recursive Subspace Bisection

First-principles molecular dynamics (FPMD) simulations of molecules, liquids and solids, are most often carried out within the framework of Density Functional Theory (DFT). When using hybrid density functionals that include the Hartree-Fock exchange energy, the computational cost increases sharply due to the need to compute $O(N^2)$ exchange integrals for N orbitals. Recursive Subspace Bisection (RSB) [F. Gygi Phys. Rev. Lett. 102, 166406 (2009)] provides a compact representation of orbitals, leading to a large acceleration of the computation of exchange integrals while preserving controlled accuracy. We present results of hybrid DFT simulations carried out using the RSB approach and demonstrate the performance of this approach in inhomogeneous systems in which orbitals have varying localization properties [W. Dawson and F. Gygi, J. Chem. Theory Comput. 11, 4655 (2015)].

Francois Gygi
University of California, Davis
fgygi@ucdavis.edu

MS15

A Posteriori Quantification of Model/discretization/solution Method Errors for Electronic Structure Calculations

Ab initio methods, based on first principles are more and more appreciated for the numerical simulation of electronic structures. Starting from the Schrödinger equations, under the Born Oppenheimer assumption, the solution Ψ which is a function of x representing the position in $\mathbb{R}^{3N}$ of the N electrons of the system. This problem is of course out of reach currently at least for complex molecules and simplifications based on further modeling is needed. There are essentially two families of approaches: the Kohn-Sham approach the solution of which is the electron density. The development of improved models is still an active research area. The second family of approaches is based on various generalizations of the Hartree Fock frame such as post Hartree Fock that allow to increase their accuracy. In this presentation we focus on this second family and provide a posteriori error estimates that allow to balance the errors due to i) the model post Hartree Fock approximation versus Schrödinger, ii) the discretizations based on the choice and size of basis set and iii) solution errors either at the level of linear algebra or fixed point (SCF) incomplete iterations. This work summarizes the contributions of E. Cances, G. Dusson, F. Lipparini, B. Stamm, M. Vohralik

Yvon Maday
Universite Pierre et Marie Curie
and Brown university
maday@ann.jussieu.fr

MS15

Improving Density Functional Theory for Warm Dense Matter

Warm dense matter is a high-energy state of matter with characteristics of both solids and plasmas. It is found within planetary interiors, created during shock experiments, and observed along the path to ignition of inertial confinement fusion. The effects of these environments' high temperatures and pressures demand a mixed quantum-classical treatment. Due to this complicated behavior, simulation of warm dense matter is notoriously challenging for both condensed matter and traditional plasma methods. One of the most successful methods for modeling warm dense matter to date uses density functional theory to describe the electrons within a material and classical molecular dynamics to describe its ions. We know, however, that this treatment ignores an important piece of the electronic energy's explicit temperature dependence. In this talk, ensemble and other temperature effects on static and time-dependent electronic structure are examined through the lens of mathematical density functional theory. In addition, a new method uniquely suited to warm dense matter simulation will be presented: finite-temperature potential functional theory. Highly accurate, systematically improvable, and computationally efficient, it bridges the theoretical gap between condensed matter and plasma treatments and skirts the computational bottleneck of high-temperature density functional theory.

Aurora Pribram-Jones
University of California, Irvine
apribram@uci.edu

MS16

Bounds on Stieltjes Functions and Their Applications to Passive Cloaking

In this talk, we derive bounds on Stieltjes functions which generalize those provided by M. Gustafsson and D. D. Sjberg and apply them in the context of broadband cloaking to negatively answer the following question. For the quasi-static approximation of Maxwell's equation, is it possible to construct a passive cloaking device that will cloak an object over a whole frequency band?

Maxence Cassier
Assistant Professor and Lecturer in Mathematics
Department of Mathematics, University of Utah
cassier@math.utah.edu

Graeme Milton
Distinguished Professor of Mathematics
Department of Mathematics University of Utah
milton@math.utah.edu

MS16

Complex Analysis and Herglotz Functions in the Mathematics of Sea Ice

Integral representations for Herglotz functions have been

very useful in studying the effective, homogenized properties of sea ice, a composite of ice with brine inclusions. Such properties include the effective complex permittivity of sea ice viewed as a two phase composite, or viewed as a polycrystalline composite, and the effective thermal conductivity in the presence of a brine velocity field. On much larger scales representations for Herglotz functions arise in studying the effective diffusivity of a buoy on an ice floe diffusing in the pack under the influence of oceanic and atmospheric flows. In this lecture I will discuss various Herglotz representations and their applications to sea ice.

Kenneth Golden
Professor of Mathematics
Department of Mathematics University of Utah
golden@math.utah.edu

MS16

Herglotz Functions and Sum Rules for Passive Systems

The connection between passive system, Herglotz (or positive real) functions, sum rules, and physical bounds are reviewed. Physical bounds are determined from sum rules that relate the low and high-frequency asymptotic expansion of a Herglotz function with its dynamic response. The sum rules and physical bounds are compared with numerical and experimental results for; broadband matching, absorbers, high-impedance surfaces, temporal dispersion of metamaterials, periodic structures, scatterers, extraordinary transmission, and antennas.

Mats Gustafsson
Professor of Electromagnetic Theory, Department
of Electrical and Information Technology Lund Uni
mats.gustafsson@eit.lth.se

MS17

Modelling and Simulation of Magnetic Fluids

Abstract not available

Hector D. Ceniceros
Department of Mathematics
University of California Santa Barbara
hdc@math.ucsb.edu

MS17

A Coupling Strategy for Nonlocal and Local Models with Mixed Volume Constraints and Boundary Conditions

We present an optimization-based coupling of local and nonlocal continuum models. The coupling is formulated as a control problem where the states are the solutions of the nonlocal and local equations, the objective is to minimize their mismatch on the overlap of the local and nonlocal domains, and the controls are volume constraints and boundary conditions. We present numerical results illustrating the accuracy and efficacy of the method in the context of nonlocal diffusion and nonlocal elasticity.

Marta D'Elia
Sandia National Laboratories
mdelia@sandia.gov

MS17

Traction Boundary Conditions for Molecular Static Simulations

In this talk, we will discuss an approach to impose traction boundary conditions (TBC) for atomistic models. This is a nontrivial task due to the atomistic interaction beyond the nearest neighbor. We will discuss the derivation of such boundary conditions in the 1D case, their stability and continuum limit, and extension to higher dimensions.

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

MS17

Recent Development of Numerical Methods on Finding Saddle Point and Minimum Energy Path

The dynamics of complex systems is often driven by multiscale, rare but important events. Finding saddle point and minimum energy path on an energy surface has attracted much attention in various areas such as nucleation in phase transition, chemical reaction, biology, etc. In this talk, I will present some recent progress on two different numerical algorithms: 1) Optimization-based shrinking dimer method, which reformulates the classical dimer method under an optimization framework. We then apply the Barilai-Borwein gradient method to achieve superlinear convergence; 2) Adaptive step-size string method, which treat the original string method as an iteration process to minimize the Friedlin-Wentzell functional. We demonstrate that the Friedlin-Wentzell action can reveal how far from a general path to an MEP so that we can prove the adaptive step-size string method locally converges to the MEP.

Lei Zhang
Peking University
Beijing International Center for Mathematical Research
zhangl@math.pku.edu.cn

MS18

Jammed Packings on Arrested Emulsion Droplets

Particle packings in ellipsoidal arrested emulsion droplets are studied by computer simulation. A combination of linear programming and energy minimization techniques are used to assess the stability of these packings. By successively unjamming an arrested configuration and further relaxing the surface, the packing approaches a new "metric jammed" state stable with respect to both particle position and surface evolution. The relationship between metric jamming and classical jamming in euclidean space are discussed.

Christopher J. Burke
Tufts University
christopher.burke@tufts.edu

Timothy J. Atherton
Tufts University
Department of Physics
timothy.atherton@tufts.edu

MS18

Universal Slip Statistics: From Nanocrystals to Earthquakes

The deformation of many solid and granular materials is not continuous, but discrete, with intermittent slips similar

to earthquakes We show that the statistical distributions of the slips, such as the slip-size distributions, and the temporal slip profiles, reflect tuned criticality, with approximately the same regular (power-law) functions, and tunable exponential cutoffs, for systems spanning 13 decades in length, from nanometers to kilometers, for compressed nano-crystals, amorphous materials, sheared granular materials, lab-sized rocks, and earthquakes. The similarities are explained by a simple analytic model, which suggests that results are transferable across scales. This model provides many new predictions for future experiments and simulations. The studies draw on methods from the theory of phase transitions, the renormalization group, and numerical simulations. Connections to other systems are discussed.

Karin Dahmen
University of Illinois, Department of Physics
dahmen@illinois.edu

MS18

Inter-Particle Force Inference in Opaque Granular Materials Imaged Using X-Ray Tomography and Diffraction

We describe the results of quantitative inter-particle force inference in an assembly of 77 quartz grains imaged using 3D X-ray tomography and diffraction. The results elucidate the evolution of forces and their chain-like structures during a load-unload cycle in the bulk of a stiff opaque material. We discuss the statistics of these forces and examine their heterogeneous nature as a function of macroscopic load. We also discuss future implications for grain scale modeling.

Ryan C. Hurley
Mechanical and Civil Engineering
Caltech
rchurley@gmail.com

Stephen Hall
Lund University
stephen.hall@solid.lth.se

Jose Andrade
California Institute of Technology
jandrade@caltech.edu

Jonathan Wright
European Synchrotron Radiation Facility
wright@esrf.fr

MS18

How Do Hard-Sphere Colloidal Glasses Respond to Deformation?

We investigate the microscopic and macroscopic responses of an amorphous material to deformation by performing experiments on 3D hard-sphere colloidal glasses. We measure the individual particle trajectories of tens of thousands of individual colloidal particles in a glass over time under conditions of either quiescence or applied strain. For the deformation experiments, we apply macroscopic shear to a maximum applied strain, then reverse the deformation until the bulk strain returns to zero. The particle positions over time provides a discrete sampling of the local deformation and strain in the glass, which we use to investigate the local material response to deformation.

Katharine E. Jensen
Engineering and Applied Science
Yale University
katharine.jensen@yale.edu

MS19

Deformation and Yielding in Soft Solids

Self-assembly and aggregation of soft condensed matter (proteins, colloids or polymers) into poorly connected and weakly elastic solids is very common and ubiquitous in nature. Phase separation, spinodal decomposition as well as externally driven self-assembly or aggregation often lead to gels, which display a variety of structural and mechanical features. In most cases, the interaction energies and the size of the aggregating units make these structures quite sensitive to thermal fluctuations, with a rich relaxation dynamics associated to spontaneous and thermally activated processes. In addition to affecting the aging of the material properties at rest, those dynamical processes interplay with an imposed mechanical load or deformation and are hence crucial for the mechanical response of this class of solids. I will discuss how new insight can be gained using a minimal model and numerical simulations to analyze the cooperative dynamics emerging from the microstructure of the material and its mechanical response to shear deformations.

Emanuela Del Gado
Georgetown University
ed610@georgetown.edu

MS19

Simple Approach of Stress Diffusion in Shear Banding

Session code: AB; oral; yes, can transfer to poster. Complex fluids, such as polymer systems, may exhibit separation into bands when they are sheared, each band undergoing a different shear rate. The banding stress and shear rates do not depend on the applied shear rate. This behavior is expected for a non-monotonic flow curve (shear stress-shear rate relation for homogenous shear flow). It has been shown that stress 'diffusion, when added to the constitutive model, can capture these experimental results. Here, we derive a simple origin of stress 'diffusion' due to polymer stiffness, which leads to non-linear couplings. We apply it to the Johnson-Segalman model and compare it to models proposed in the literature.

Elian Masnada, Peter Olmsted
Georgetown University
elian.masnada@gmail.com, peter.olmsted@georgetown.edu

MS19

Mesoscopic Modeling of Networked Fluids

Networked fluids, such as wormlike micellar solutions, are studied through either macroscopic models or direct mesoscopic simulation. In this talk, we model and simulate a transiently networked system at the mesoscale level based on earlier work of van den Brule in which the network is simulated with clear physical rules. This approach allows the network to relax globally due to local disentanglements and allows a direct relationship between a network connec-

tors length and its stress.

Lin Zhou
Mathematics Department, New York City College of Techonology
Brooklyn, NY 11201, USA
lzhou@citytech.cuny.edu

L. Pamela Cook
Dept of Mathematical Sciences
U of Delaware
cook@math.udel.edu

MS19

Mesoscopic Modelling of Viscoelastic Properties of Micellar Solutions

We have succeeded in extending the early works on wormlike micelles by including recent advances of polymer theories. Using a novel fast pointer algorithm that we developed, our new model allows, for the first time, quantitative prediction of experimental flow behaviors for micellar solutions with a range of concentrations of surfactant, salt, and other solution components, which is of great importance in design and characterization of wormlike micelle solutions for different applications.

Weizhong Zou
University of Michigan
weizhong@umich.edu

Ronald Larson
Department of Chemical Engineering
University of Michigan, Ann Arbor
rlarson@umich.edu

Xueming Tang
University of Michigan
xueming@umich.edu

Mike Weaver, Peter Koening
The Procter & Gamble Company
weaver.mr@pg.com, koenig.ph@pg.com

MS20

Mesoscale Model of Reaction Front Propagation in Heterogeneous Condensed Systems

Session Code W Reaction initiation and propagation in solid-state systems is investigated. We develop a macroscopic model of reaction propagation that takes into account thermal and chemical heterogeneities of the reacting media. Then, we apply this model to examine the effect of the material chemical heterogeneity on the reaction wave propagation in the mechanically activated composites. The results of computations indicate that the reaction propagates as a discrete combustion wave exhibiting pulsating temperature front oscillations.

Yuriy Gulak, Alberto Cuitino
Department of Mechanical & Aerospace Engineering
Rutgers, The State University of New Jersey
ygulak@jove.rutgers.edu, cuitino@jove.rutgers.edu

MS20

Information-Theoretic Tools for Coarse-Graining of Non-Equilibrium Systems

We present a variational approach yielding optimized coarse-grained molecular models for both equilibrium and non-equilibrium molecular dynamics. The approach can compare microscopic behavior of molecular systems to parametric and non-parametric coarse-grained models using the relative entropy between distributions on the path space and setting up a corresponding path-space variational inference problem. We present generalizations of force-matching methods with path-space information methods, and demonstrate enhanced transferability of information-based parameterizations to general observables using information inequalities.

Markos A. Katsoulakis
University of Massachusetts, Amherst
Dept of Mathematics and Statistics
markos@math.umass.edu

Petr Plechac
University of Delaware
Department of Mathematical Sciences
plechac@math.udel.edu

MS20

Fronts and Patterns in Surface Reaction-Diffusion Systems from Molecular-Level Modeling: CO Oxidation on Metals

Applications of lattice-gas (LG) models to real-world surface reaction-diffusion systems have progressed significantly with the help the density-functional theory (DFT). Quantitative agreements with experiments can be achieved through kinetic Monte Carlo simulations of multi-site (ms) LG models using DFT derived parameters. For the mesoscopic diffusion process, transport coefficients are derived from fluctuations using Einstein relation. This heterogeneous msLG approach is used to elucidate non-MF behavior in reaction fronts observed for catalytic CO oxidation on metals.

Da-Jiang Liu
Ames Lab DOE
dajiang@fi.ameslab.gov

Jim W. Evans
Ames Laboratory USDOE and Iowa State University
evans@ameslab.gov

MS20

First Principles Prediction of Optimal Catalyst Active Site

An impactful avenue of multiscale simulation is the prediction of new materials. We will demonstrate how descriptor-based modeling can enable such a search. We will demonstrate this methodology for the ammonia decomposition on bimetallic catalysts using first principles kinetic Monte Carlo (KMC) simulations. We will show that the microstructure of materials plays a profound role and poses interesting optimization problems.

Dion Vlachos
University of Delaware

vlachos@che.udel.edu

MS21

Sensitivity Analysis of the Reaxff Potential Parameter-Space

The ReaxFF potential is a complex functional formulated to synergistically describe different interatomic interaction. These set of functions are comprised of many fitting parameters. How these parameters affect the resulting force field is not well understood. We applied OFAT and LHS experimental designs in order to study the sensitivity of boron carbides' structural properties to fitting parameters. These approach allows an optimal and more sensible methodology for parameterizing ReaxFF.

Efrain Hernandez, Shawn Coleman, Mark Tschopp
Army Research Laboratory
efrain.hernandez18.ctr@mail.mil,
shawn.p.coleman8.ctr@mail.mil,
mark.a.tschopp.civ@mail.mil

MS21

A Coarse-Grained and Time Accelerated Modeling for Protein Unfolding Dynamics

We present a new mulitscale modeling of protein unfolding process by combining the coarse-grained description of proteins with time accelerated dynamics. The collective variables for proteins are extracted based on the dynamic elastic network model (DENM) [M. Deng and G. Karniadakis, 2014], where the protein interaction network and its potentials are constructed based on information of its native-state structure. The unfolding process is accelerated by the method of temperature-accelerated molecular dynamics (TAMD) [G. Abrams and E. Vanden-Eijnden, 2010]. The unfolding process is mimicked by a series of jump events of overcoming the local energy barrier on the free energy landscape with force loading. The jumping events from local energy minima (bonds breaking rate) are chosen according to Kramers theory and the Bell model. We compare the simulations from the new multiscale method with those from fully atomistic Molecular Dynamics by studying the force-extension process of the Fibrinogen and Titin Immunoglobulin proteins. The results confirm the robustness as well as efficiency of this new model.

Xingjie Li
university of north carolina charlotte
mathslxj@gmail.com

Mingge Deng
Division of Applied Math, Brown University
mingge_deng@brown.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

Xiu Yang
Pacific Northwest National Laboratory
xiu.yang@pnnl.gov

MS21

Predictive Coarse-Graining

We present a Bayesian formulation to coarse-graining of atomistic systems using generative probabilistic models which allows us to address the question of quantifying epistemic uncertainty. Apart from the usual coarse-grained potential that approximates the exact free energy, the formulation is augmented with a probabilistic mapping from coarse to fine, which enables the prediction of properties in the fine-scale. The formulation allows for significant flexibility and high-dimensional parameters can be learned by sparsity-enforcing priors.

Markus Schöberl
Technische Universität München
m.schoeberl@tum.de

Nicholas Zabaras
The University of Warwick
Warwick Centre for Predictive Modelling (WCPM)
nzabaras@gmail.com

Phaedon S. Koutsourelakis
Technische Universität München, Germany
p.s.koutsourelakis@tum.de

MS21

Polymer Looping: Kinetics and Mean First Passage Time

The Rouse and Zimm models have been thoroughly used to study the loop closure problem for homogeneous polymer chains. We present loop closure time estimates for generalizations of these popular models to polymers with inhomogeneities in the monomer properties.

Panos Stinis
Northwest Institute for Advanced Computing
University of Washington
panagiotis.stinis@pnnl.gov

MS21

Adaptive Minimum Action Method for Nongradient Systems

Abstract not available

Xiaoliang Wan
Louisiana State University
Department of Mathematics
xlwan@math.lsu.edu

MS22

Homogenisation for Mean Field Games

We investigate dynamical mean field games as introduced by Lasry and Lions in the small noise limit when the Hamilton-Jacobi equation of the system has a rapidly varying dependence on the state variable x. This is joint work with Analisa Cesdaroni and Claudio Marchi.

Nicolas Dirr
Cardiff School of Mathematics
Cardiff University

dirrnp@cardiff.ac.uk

MS22

A Multiscale Damage Model in the Context of Evolutionary Gamma-Convergence

Macroscopic damage and failure phenomena of solids typically are the result of the accumulation of small cracks or defects on a microscopic scale. In engineering literature, various multi-scale or homogenized models are proposed in order to describe time-dependent damage phenomena with microscopic origins like the growth of microcracks or micro-voids. In this lecture, we discuss these approaches in the framework of homogenization and evolutionary Gamma-convergence, allowing for micro-defects that may grow individually with respect to the time-dependent loadings. The lecture relies on joint work with Hauke Hanke (Berlin).

Dorothee Knees
Institute for Mathematics
Universität Kassel, Germany
dknees@mathematik.uni-kassel.de

MS22

Homogenization in Fractional Elasticity

We consider a visco-elastic material with constitutive relations involving fractional-in-time derivatives with oscillating coefficients and address the effective behavior of the material law for the asymptotic limit of infinitely large oscillations. The limit material model admits a series representation with infinitely many fractional derivatives. Formulas can be made explicit for the $1+1$-dimensional case with periodic coefficients. The results can be found in [W, Homogenization in fractional elasticity, SIAM J Math Anal 46(2): 1551–1576, 2014].

Marcus Waurick
Department of Mathematical Sciences
Univeristy of Bath, UK
marcus.waurick@tu-dresden.de

MS23

Materials Studies by the Bilbao Crystallographic Server

The **Bilbao Crystallographic Server** (www.cryst.ehu.es) is a free web site with crystallographic databases and programs. The databases give access to crystallographic data of space and point groups, magnetic space groups, subperiodic groups, their representations and group-subgroup relations. Specialized software facilitates the studies of wide range of complex solid-state physics and structure-chemistry problems like pseudosymmetry, crystal-structure relationships, prediction of new ferroic and multiferroic materials, *etc.* Illustrative examples will demonstrate server's capacities and efficiency in materials-science studies.

Mois I. Aroyo, J.Manuel Perez-Mato, Luis Elcoro, Samuel Gallego, Gemma de la Flor
Fsica de la Materia Condensada
Universidad del Pas Vasco
mois.aroyo@ehu.es, jm.perez-mato@ehu.es,
luis.elcoro@gmail.com, twmpatd@gmail.com,
gemma.delaflor@ehu.es

Emre Tasci
Department of Physics Engineering
Hacettepe University
emre.tasci@hacettepe.edu.tr

Gotzon Madariaga
Fsica de la Materia Condensada
Universidad del Pas Vasco
gotzon.madariaga@ehu.es

MS23

The 12 Spheres Problem

This talk describes the long history and current state of knowledge, theoretically and computationally, about the configuration space of 12 non overlapping spheres of radius r constrained to touch a fixed sphere of radius 1. We consider how the topology of the configuration space changes with the radius, the value of the maximal radius, and the connectivity of the space. We also treat smaller numbers of spheres.

Jeffrey Lagarias
Dept. of Mathematics
University of Michigan
lagarias@umich.edu

Robert Kusner
Dept. of Mathematics and Statistics
Univ. of Massachuesetts, Amherst
robkusner@gmail.com

Woden Kusner
Institut for Analysis and Number Theory
Graz Univ. of Technology, Graz, AUSTRIA
wkusner@gmail.com

Senya Shlosman
Aix-Marseille University, Universite de Toulon
CNRS, Marsielles, FRANCE
senya.shlosman@univ-amu.fr

MS23

Applications of Groupoids to the Description and Interpretation of Crystal Structures: The Example of Pyxorenes

The structures of pyroxene polymorphs can be described as cell-twins based on a common layer consisting of half the unit cell of clinoenstatite. The cell-twin operations are partial operations belonging to a special case of space groupoid which was called twinned space group in the pioneering studies by Ito started in 1935. The groupoid analysis of pyroxene polymorphs is presented and the special place they occupy in the category of polytypes is discussed.

Massimo Nespolo
Cristallographie, Résonance Magnétique et Modélisations
UMR CNRS 7036 Université de Lorraine
massimo.nespolo@crm2.uhp-nancy.fr

Mois I. Aroyo
Fsica de la Materia Condensada
Universidad del Pas Vasco

mois.aroyo@ehu.es

MS23

Recognizing the Lattice Type to Which a Unit Cell (almost) Belongs

Minisymposium Session Code:N,O,P,Q Oral Presentation We propose a new approach for comparing unit cells and the corresponding lattices which is based on general purpose lattice reduction techniques (in particular LLL-reduction). This approach not only allows to efficiently quantify the similarity between two lattices, it can also be used to detect pseudo-symmetry of lattices by showing that a given unit cell is close to one having higher symmetry.

Bernd Souvignier
IMAPP Institute for Mathematics, Astrophysics and Particle Physics, Radboud University Nijmegen
souvi@math.ru.nl

MS24

Self-Similar Folding Patterns in Partially Delaminated Thin Films

In this talk I discuss self-similar pattern formation in a compressed elastic film that is partially delaminated from a substrate. Such patterns were observed in recent experiments to fabricate nanochannels from semiconductor films. By proving rigorous upper and lower bounds on the minimum value of a suitable energy functional we predict the patterns observed in experiments.

David P. Bourne
Durham University
David.Bourne@durham.ac.uk

Sergio Conti
Institut fur Angewandte Mathematik
Universitat Bonn
sergio.conti@uni-bonn.de

Stefan Mueller
University of Bonn
stefan.mueller@hcm.uni-bonn.de

MS24

Brittle Linearly Elastic Thin Films

We present a rigorous derivation of a Kirchhoff-Love Griffith model for the initiation and propagation of cracks in a thin film under quasistatic loading. Previous studies (by Braides-Fonseca, Bouchitt-Fonseca-Leoni-Mascarenhas, Babadjian, Freddi-Paroni-Zanini) considered scalar-valued problems, coercivity assumptions incompatible with 3D elasticity, or cracks with pre-specified paths and geometries. The main difficulty in the vectorial case is to establish a compactness result on minimizing sequences, showing the structure of limit displacements and cracks with finite energy. We show how to do this using tools from geometric measure theory and fine properties of bounded deformation functions.

J.-F. Babadjian
Laboratoire Jacques-Louis Lions (UMR-CNRS 7598)
Université Paris 6 (UPMC)
babadjian@ann.jussieu.fr

Duvan Henao
Pontificia Universidad Catolica de Chile
dhenao@mat.puc.cl

MS24

A Variational Model for Fracture and Debonding of Thin Films Under In-Plane Loadings

We study fracture and debonding of a thin film bonded to a rigid substrate through a thin compliant layer, introducing a two-dimensional variational fracture model. Fractures are distinguished between codimension-1 (cracks in the film) and codimension-0 (interfacial debonding) discontinuity sets. In order to study the mechanical response of such systems under increasing loads, we formulate a rate-independent irreversible evolution law accounting for both transverse fracture and debonding. We justify the dimension reduction model in the setting of scalar-valued displacement fields by a variational asymptotic analysis, starting from the three-dimensional variational fracture problem under scaling hypotheses on material and geometric parameters. We propose a numerical implementation based on a regularized formulation of the fracture problem via a gradient damage functional, explore the emergence of crack patterns, providing qualitative comparison with real life examples.

Andrés A León Baldelli
Mathematical Institute
University of Oxford
leonbaldelli@maths.ox.ac.uk

J.-F. Babadjian
Laboratoire Jacques-Louis Lions (UMR-CNRS 7598)
Université Paris 6 (UPMC)
babadjian@ann.jussieu.fr

B. Bourdin
Dept. of Mathematics and Center for Computation & Technology
Louisiana State University
bourdin@math.lsu.edu

D. Henao
Facultad de Matemáticas
Pontificia Universidad Católica de Chile
dhenao@mat.puc.cl

C. Maurini
Institut Jean Le Rond d'Alembert (UMR-CNRS 7190)
UPMC
Institut Jean Le Rond d'Alembert (UMR-CNRS 7190)
CNRS
corrado.maurini@upmc.fr

MS25

Grain Growth in Metallic Films: Simulations and Experiments

Experimental grain growth characteristics are examined for Al and Cu films. The experimental data set is used to evidence stagnation of grain growth and arrive at a universal size distribution. This distribution differs from the distribution obtained in two-dimensional simulations of grain growth with isotropic boundary energy. Surface and elastic strain energy, anisotropy of boundary energy, grooving, impurity drag, and triple-junction drag are examined as the causes of the observed difference between experiment

and simulation.

Katayun Barmak
Department of Applied Physics and Applied Mathematics
Columbia University
kb2612@columbia.edy

MS25

Convergence of Thresholding Schemes for Mean-Curvature Motion

The thresholding scheme, a time discretization for mean-curvature flow was introduced by Meriman, Bence and Osher in 1992. In the talk we present new convergence results for several variants of this scheme, in particular in the multi-phase case with arbitrary surface tensions. Our proof is similar to the convergence results of Almgren, Taylor and Wang in 1993 and Luckhaus and Sturzenhecker in 1995 using the gradient flow structure of mean curvature flow.

Tim Laux
Max Planck Institute
Leipzig, Germany
tim.laux@mis.mpg.de

Felix Otto
Max Planck Institute for Mathematics in the Sciences
Leipzig, Germany
Felix.Otto@mis.mpg.de

Drew Swartz
Booz Allen Hamilton
Washington D. C.
drew.e.swartz@gmail.com

MS25

Growth of Grain Boundary Grooves by Anomalous Surface Diffusion

It has been recognized recently that the diffusion on the solid surface is anomalous in many cases, including adsorbed nanocrystals, nanoscale direct deposition processes, and bulk-mediated surface diffusion. In the present talk, we consider the groove growth in the cases of surface superdiffusion and surface subdiffusion. In each case, an exact self-similar solution is obtained, and basic properties of the solution are described.

Alexander Nepomnyashchy
Department of Mathematics
Technion
nepom@techunix.technion.ac.il

Mohammad Abu Hamed
Technion - Israel Institute of Technology
mohammad@techunix.technion.ac.il

MS25

Surface Effects on Grain Boundary Migration in Thin Films

To gain insight into the effects of the exterior surface on grain boundary migration, we consider thin film axisymmetric two grain geometries with bamboo structure. If the system is of infinite extent, there do not exist nontrivial steady states. However steady states do exist in finite systems, and their relative energies may be calculated. We conjecture that steady states can mimic slowly varying features in larger systems. Some results of numerical simulations are presented.

Amy Novick-Cohen
Technion Israel Institute of Technology
amync@tx.technion.ac.il

John McCuan
Dept of Mathematics
Georgia Tech
mccuan@math.gatech.edu

Arkady Vilenkin
Hebrew University of Jerusalem
vilenkin@vms.huji.ac.il

MS26

Algorithms for Large-Scale All-Electron Density Functional Theory and Beyond

This talk summarizes new developments towards efficient, accurate all-electron electronic structure theory for total energies and excited states of materials and molecules, specifically: (i) A new, general electronic structure infrastructure "ELSI" that integrates approaches to help overcome the Kohn-Sham eigenvalue solver bottleneck. (ii) More accurate basis set recipes for explicitly correlated ground state calculations, and for excited state calculations using G0W0 and linear response TD-DFT.

Volker Blum
Duke University
Department of Mechanical Engineering and Materials Science
volker.blum@duke.edu

MS26

Large-Scale Real-Space All-Electron Kohn-Sham Density Functional Theory Calculations

We present a computationally efficient method to perform large-scale all-electron Kohn-Sham density functional theory calculations by enriching the Lagrange polynomial basis in classical finite element (FE) discretization with atom-centered numerical basis functions (enrichment functions), which are obtained from the solutions of the Kohn-Sham (KS) problem for single atoms. We demonstrate the accuracy, efficiency and scalability of the proposed method on various metallic and insulating benchmark systems, with systems ranging in the order of 10,000 electrons. We observe a 50-100 fold reduction in the overall computational time when compared to classical FE calculations while being commensurate with the desired chemical accuracy.

Bikash Kanungo
University of Michigan
bikash@umich.edu

Vikram Gavini
Mechanical Engineering, University of Michigan
vikramg@umich.edu

MS26

The Flexibility of Daubechies Wavelets for Electronic Structure Calculations

In recent works, we presented the linear scaling version of

the BigDFT code based on Daubechies wavelets, where a minimal set of localized support functions is optimized in situ. Our linear scaling approach is able to generate support functions for systems in various boundary conditions, like isolated, surface and periodic, and it is based on a algorithm which is universally applicable, requiring only moderate amount of computing resources. We will present how the flexibility of this approach is helpful in providing a basis set that is optimally tuned to the chemical environment surrounding each atom. In addition than providing a basis useful to project Kohn-Sham orbitals informations like atomic charges and partial density of states, it can also be reused as-is, i.e. without reoptimization, for charge-constrained DFT calculations within a fragment approach. We demonstrate the interest of this approach to express highly precise and efficient calculations for the computational setup of systems in complex environments.

Luigi Genovese
Institut Nanosciences et Cryogénie, CEA
luigi.genovese@cea.fr

MS26

Fast Electronic Structure Calculation Methods for Studying Low-dimensional Nanomaterials

Low-dimensional materials such as graphene and phosphorene nanoribbons and nanoflakes exhibit intriguing phenomena. Their electronic properties depend on how they are cut from bulk materials, i.e., their edge types, how edges are passivated, the presence of defects, and their sizes. Efficient and reliable computational tools must be used to study these nanomaterials, which can contain more than 10,000 atoms, in a systematic fashion. We discuss a number of recent algorithmic advances that enable these studies.

Chao Yang
Lawrence Berkeley National Lab
cyang@lbl.gov

MS27

Matrix Pade Approximants of Stieltjes Functions

The spectral measure in the Stieltjes integral representation of the effective properties of a composite contains all information about the microstructure and can be uniquely recovered from effective measurements known in an interval of frequency. We consider a case of matrix valued measure corresponding to anisotropic composites. Matrix Pade approximants are constructed using matrix polynomials orthogonal with respect to the spectral measure. We discuss applications to inverse homogenization and to numerical simulation of wave propagation in composite materials.

Elena Cherkaev
Professor of Mathematics
Department of Mathematics University of Utah
elena@math.utah.edu

MS27

Determination of Optimal Performance of Electromagnetic Devices Using Convex Optimization

Various electromagnetic devices like antennas, filters, transmission lines etc can be characterized in terms of Herglotz functions, and can thus be represented by a measure (the imaginary part on the real line). By discretizing this measure we can use convex optimization to investigate how close a response function can come to an arbitrarily specified goal function, and the associated cost. This can sometimes be interpreted in physically relevant quantities, like minimum required physical size.

Daniel Sjöberg
Professor of Electromagnetic Theory
Lund University
daniel.sjoberg@eit.lth.se

MS27

Analyticity of the Dirichlet-to-Neumann Map for Maxwell's Equations in Passive Composite Media

In this talk I will discuss the analyticity properties of the electromagnetic Dirichlet-to-Neumann (DtN) map for the time-harmonic Maxwell's equations for passive linear multicomponent media and the connection of this map to Herglotz functions. The properties of the DtN map are derived in terms of the transfer matrix for layered media and, for bounded media, using a variational formulation of Maxwell's equations. This is joint work with Graeme Milton and Maxence Cassier (Univ. of Utah).

Aaron Welters
Assistant Professor of Mathematical Sciences
Florida Institute of Technology
awelters@fit.edu

Maxence Cassier
Assistant Professor and Lecturer in Mathematics
Department of Mathematics, University of Utah
cassier@math.utah.edu

Graeme W. Milton
University of Utah
Department of Mathematics
milton@math.utah.edu

MS28

Embedded Corrector Problem and Boundary Integral Methods for Stochastic Homogenization

A very efficient algorithm has recently been introduced in order to approximate the solution of implicit solvation models for molecules. The main ingredient of this algorithm relies in the clever use of a boundary integral formulation of the problem to solve. The aim of this talk is to present how such an algorithm can be adapted in order to compute efficiently effective coefficients in stochastic homogenization for random media with spherical inclusions. To this aim, the definition of new approximate corrector problems and approximate effective coefficients is needed and convergence results in the spirit are proved for this new formulation. Some numerical test cases will illustrate the behaviour of this method.

Virginie Ehrlacher
CERMICS - Ecole des Ponts Paristech / INRIA
ehrlachv@cermics.enpc.fr

Eric Cances
Ecole des Ponts and INRIA, France
cances@cermics.enpc.fr

Benjamin Stamm
University of California, Berkeley, US
stamm@math.berkeley.edu

Frederic Legoll
LAMI, ENPC
legoll@lami.enpc.fr

MS28

Variational Analysis of a Quasicontinuum Method

We study the validity of a quasicontinuum (QC) method from a modeling point of view using variational techniques. The system we consider is a one-dimensional chain of atoms with finite range interactions of Lennard-Jones type. On the one hand we study the fully atomistic model as the number of atoms becomes large. On the other hand we analyze the asymptotic behavior of a corresponding QC model. A comparison shows that there is an immediate coincidence in the regime of elasticity, while the asymptotic expansions of the two models differ in the case of fracture. However, we show that the minimal energies and the minimizers are the same if the discretization in the continuum region of the QC model is chosen coarse enough. This is extending earlier results for nearest and next-to-nearest neighbor interactions to finite range interactions. For the former see: M. Schffner, A. Schlmerkemper, On a Gamma-convergence analysis of a quasicontinuum method, Multiscale Model. Simul. 13, 132–172 (2015).

Anja Schlömerkemper
University of Würzburg
anja.schloemerkemper@mathematik.uni-wuerzburg.de

Mathias Schäffner
TU Dresden
mathias.schaeffner@tu-dresden.de

MS28

Application of the Multiscale Micromorphic Molecular Dynamics for Nanoindentation of Silicon

Session Code: E; Oral; Yes, you can transfer to poster In this work, we applied the recently developed Multiscale Micromorphic Molecular Dynamics (MMMD) to simulate nanoindentation of single crystal silicon. The main advantage to employ the MMMD method to simulate nanoindentation of Silicon is to accurately capture the dislocation induced twinning and structure phase transformation for finite size single crystal specimens. The MMMD method provides a multiscale transition from molecular dynamics to continuum mechanics.

Shingo Urata
Asahi Glass Co., Ltd.
University of California Berkeley
shingo-urata@berkeley.edu

Shaofan Li
University of California Berkeley
shaofan@berkeley.edu

MS28

Simulations of Material Interface Problems Using Atomistic-Based Boundary Element Method

We consider the atomistic/continuum coupling problems in the dynamics setting. Of particular interest is the interaction of stress waves and local lattice defects. There are several modeling issues. First, the phonon waves generated by the local defects need to propagate out of the atomistic region without being reflected. On the other hand, external elastic waves need to enter the atomistic regions, which will lead to the migration of the defects. These two processes will occur many times. The empirical approach of introducing damping terms will not address these two issues at the same time. The third issue is that in realistic systems, there are many local defects, and the entire physical domain is at least at the micron scale. The leads to a continuum region with complex geometry. I will present a boundary element framework, derived directly based on the underlying molecular dynamics model, to address all these critical issues. As examples, we present some results on fracture simulations, where micron-scale systems can be simulated with a much reduced cost.

Xiaojie Wu
Penn State University
xxw139@psu.edu

MS29

Arresting Relaxation in Pickering Emulsions

Pickering emulsions are mixtures of immiscible fluids stabilized by the presence of colloidal particles. Non-spherical emulsion droplets can be sculpted by a general mechanism of deformation, absorption of particles, relaxation of the droplet and arrest in a non-equilibrium shape. In this talk, I will present a detailed study of the microsctructure of arrested packings that uncovers the relative influence of geometry and dynamics; the connection between arrest and jamming will also be discussed.

Timothy J. Atherton
Tufts University
Department of Physics
timothy.atherton@tufts.edu

MS29

Homogenization of Defects: The Emergence of Torsion and Non-Metricity

Session code: AA; Oral; No, transfer to poster. The modeling of defects in solids has a long ongoing history. One approach, which goes back to the early 1900s, views defects as geometric singularities in locally-Euclidean manifolds. Another approach, dating from the 1950s, models continuously-distributed defects as smooth manifolds endowed with extra fields representing the defects. In this lecture, the two approaches are reconciled. It will be shown that the continuum models of defects are genuine limits of singular defects as their density tends to infinity. By introducing a new notion of weak convergence, we show how torsion arises as a homogenization limit of manifolds with distributed singular dislocations, and similarly, how non-metricity arises a homogenization limit of manifolds with distributed point defects.

Raz Kupferman
Institute of Mathematics,
The Hebrew University
raz@math.huji.ac.il

MS29

Shape Formation in Plates with Incompatible Pre-Strains

In this talk we will review a class of design problems in solid mechanics, leading to a variation on the classical question of equi-dimensional embeddability of Riemannian manifolds. In this general context, we will be concerned

with: (1). The variational formulation of the inverse design problem and establishing bounds on the energy infimum corresponding to the deformations of low regularity, obtained through convex integration techniques applied to the effective constraint equations. (2). Deriving the necessary and sufficient integrability conditions of the studied problems. (3). Studying the dimension reduction 3d to 2d in different energy scaling regimes. This talk will be based on results obtained in collaboration with Amit Acharya, Reza Pakzad, Annie Raoult and Diego Ricciotti.

Marta Lewicka
Department of Mathematics
University of Pittsburgh
lewicka@pitt.edu

MS29

The Buckling-Fracture Transition in Non-Euclidean Plates

Non-Euclidean Plates (NEP) are thin elastic plates, in which lateral equilibrium distances of the material are described by a non-Euclidean reference metric. When flattened, such materials are residually stressed. Previous studies showed that such plates buckle spontaneously while free of external constraints. In the thin limit the geometry of the buckled configurations approaches the reference metric. In this talk we show the existence of a new, buckling to fracture, transition in these plates. Depending on the parameters of the system, NEP might undergo fracture instability instead, or together with, buckling instability. We propose the scaling of this transition and verify it experimentally. Our observations lead us to propose an intrinsic geometrical description of fracture, which is consistent with, but different from Linear Elastic Fracture Mechanics.

Eran Sharon
Racah Institute of Physics
The Hebrew University
erans@mail.huji.ac.il

MS30

Mucus Microrheology as an Assay for Disease Progression and Drug Treatment

In collaborations with colleagues in the Marsico Lung Institute, a team of mathematicians and statisticians has developed methods to discern lung health versus disease on the basis of rheological properties of the lung's barrier fluid, mucus. Mucus yields at incredibly low stresses, rendering macrorheology problematic. Thus, we have pursued diagnostics on the basis of thermal fluctuations of micron-scale probes. Results from diverse mucus sources and all collaborators are discussed.

M. Gregory Forest
University of North Carolina at Chapel Hill
Dept of Math & Biomedical Engr.
forest@unc.edu

MS30

A Multiscale Model for the Thixotropic Rheology of Colloidal Suspensions

The modeling of the complex materials exhibiting structures at multiple length scales and the associated dynamical responses at multiple time scales demands the formulation of models that take into account phenomena at various levels of description. This talk describes how a population balance model together with the mesoscopic deformation dynamics of colloidal aggregates may be applied to model macroscopic thixotropic suspension rheology. Comparison with experimental data will also be discussed.

Paul Mwasame
University of Delaware
mwasamep@udel.edu

Antony N. Beris
University of Delaware
Newark, DE
beris@udel.edu

Norman Wagner
University of Delaware
wagnernj@udel.edu

MS30

A Stochastic Model of Lung Mucus Gel Networks

The viscoelastic properties of mucus inside the lungs are fundamental to our well-being. However, few mathematical models have produced significant insight into the rheology of this system. In this talk we examine the ability of elastic dumbbell models, using parallel SDEs, to capture nonlinear mucus flow by describing the breaking and reforming of entanglement points in the mucin network. This approach maintains physiologically relevant parameters necessary for the simulation of drugs or respiratory therapies.

Erik Palmer
Department of Mathematics
University of South Carolina
etpalmer@math.sc.edu

M. Gregory Forest
University of North Carolina at Chapel Hill
Dept of Math & Biomedical Engr.
forest@unc.edu

Paula A. Vasquez
University of South Carolina
paula@math.sc.edu

MS30

Modeling the Macroscopic Rheological Response of Mucin Gels Using Microscopic Polymer Network Considerations

The viscoelastic properties of mucus can primarily be attributed to the presence of large glycoproteins called mucins, which consist of protein backbones with a dense sugar sidechain bottlebrush. As a result of the inherent complexity of their biological structure, however, very little is known about the structural and dynamical details of the mucin gel which contribute to their observed bulk rheological response. It is well known, however, that the large mucins entangle and interact with each other and their surroundings via ion-mediated crosslinking and hydrogen bonding interactions, amongst others. As such, we develop a Sticky Network model in which mucin gels are modeled as an entangled network of finitely extensible dumbbells with a stretch-dependent stickiness energy parameter that must be overcome in order for the chains to be able to dissociate from the rest network. As a first example, we consider the effect of aging and degradation of saliva (for which

MUC5B in the dominant mucin) on its extensional rheology. Capillary breakup extensional rheometry (CaBER) experiments reveal that both the time to breakup and relaxation time of saliva samples decrease as a function of age. We show that our model is able to accurately capture the capillary thinning and filament rupture behaviour of saliva using biologically-derived parameters, and can account for temporal changes by simply imposing a decrease in the MUC5B molecular weight. As a second and final example, we characterize the rheological response of a variety of native and synthetic mucin gels using small amplitude oscillatory shear (SAOS) at various pH, mucin concentration, and surfactant concentration levels. We discuss how the parameters of the Sticky Network model are modified by these various environmental factors, and attempt to elucidate the effect of key mucin structural parameters on the observed rheological measurements.

Caroline Wagner, Brad Turner, Katharina Ribbeck
Massachusetts Institute of Technology
cewagner@mit.edu, bsturner@mit.edu, ribbeck@mit.edu

Gareth H. McKinley
Dept of Mechanical Engineering
Massachusetts Institute of Technology
gareth@mit.edu

MS31

Mesoscopic Simulations of Lipid Membrane Remodeling

The remodeling of lipid membranes is crucial for many biological processes, such as cell division, protein trafficking, and signaling. The remodeling process is usually facilitated by proteins, which modulate membrane dynamics. The EM2 model employs discrete quasiparticle approach to model protein-facilitated shape changes of the membrane on mesoscale length and time scales. Here, we present the newest developments in EM2 model and the most recent results of flat membrane remodeling by N-BAR proteins.

Aram Davtyan
University of Chicago
adavtyan@uchicago.edu

MS31

A Dynamic Phase-Field Model for Structural Transformations and Twinning: Regularized Interfaces with Transparent Prescription of Complex Kinetics and Nucleation

The motion of interfaces is central to structural phase transformations. Continuum models are usually regularized to allow for simple numerical calculations, but interface kinetics and nucleation is restrictive and opaque. We formulate a model with regularized interfaces that allows for transparent prescription of complex kinetics and nucleation. The key ingredients are an energy parametrization to separate nucleation from kinetics; and a conservation statement for interfaces. We present 1D and 2D calculations characterizing the formulation.

Kaushik Dayal
Carnegie Mellon University
kaushik@cmu.edu

MS31

Multiresolution of Molecular Dynamics in the Particle Domain

The length- and time-scale required for semi-crystalline materials or rare-event-phenomena involving low to medium defect concentrations, respectively, far exceed the currently computationally accessible. The problem can be resolved by reducing the number of degrees of freedom (DOFs) while increasing timesteps. The topology and sparsity of the bonding structure is used to derive a hierarchical set of DoFs providing a clear framework for full multiresolution beyond the common two-level representation.

B. Chistopher Rinderspacher
Army Research Laboratory
Macromolecular Science & Technology
berend.c.rinderspacher.civ@mail.mil

MS31

Mesoscale Modeling of Stress-Directed Compositional Patterning in Semiconductor Alloys

The ability to fabricate periodic assemblies of quantum dots on (or in) semiconductor substrates would enable a host of microelectronic and optoelectronic applications. A variable-resolution lattice kinetic Monte Carlo model is developed to predict the interdiffusion of silicon and germanium atoms in a film subjected to a pattered stress field imposed by an array of micron-scale indenters. The simulation is propagated using rates for atomic diffusion that depend on stress, composition, and temperature.

Talid Sinno
Department of Chemical and Biomolecular Engineering
University of Pennsylvania
talid@seas.upenn.edu

MS33

Norm-Resolvent Convergence of One-Dimensional High-Contrast Periodic Problems to a Kronig-Penney Dipole-Type Model

I discuss operator-norm resolvent convergence estimates for one-dimensional periodic differential operators with rapidly oscillating coefficients in the non-uniformly elliptic high-contrast setting, which has been out of reach of the existing homogenisation techniques. Our analysis is based on a special representation of the resolvent of the operator in terms of the M-matrix of an associated boundary triple, due to M. G. Kreĭn. The resulting asymptotic behaviour is shown to be described, up to a unitary equivalent transformation, by a non-standard version of the Kronig-Penney model on the real line. This is joint work with Alexander V. Kiselev.

Kirill Cherednichenko
Department of Mathematical Sciences
University of Bath, UK
k.cherednichenko@bath.ac.uk

Alexander Kiselev
National Pedagogical Dragomanov University
alexander.v.kiselev@gmail.com

MS33

Effective Maxwell's Equations in a Geometry with Flat Split-Rings

We present a result on homogenization of the time har-

monic Maxwell's equations in a complex geometry. The homogenization process is performed in the case that many (order η^{-3}) small (order η^1), thin (order η^2), and highly conductive (order η^{-3}) metallic objects are distributed in a domain $\Omega \subset \mathbb{R}^3$. We determine the effective behavior of this meta-material in the limit $\eta \searrow 0$. For $\eta > 0$, each single conductor occupies a simply connected domain, but the conductor closes to a ring in the limit $\eta \searrow 0$. This change of topology allows for an extra dimension in the solution space of the corresponding cell-problem. Even though both original materials (metal and void) have the same positive magnetic permeability $\mu_0 > 0$, we show that the effective Maxwell system exhibits, depending on the frequency, a negative magnetic response.

Agnes Lamacz
Fakultät für Mathematik
Technische Universität Dortmund, Germany
agnes.lamacz@tu-dortmund.de

MS33

Homogenization of Discrete Systems with Degenerated Growth

In this talk, we consider lattice systems with random interactions between the lattice points. We assume that the interaction potentials satisfy growth conditions which are degenerated and are given in terms of certain weight functions. We show that under suitable integrability assumptions for the weight functions and stationarity/ergodicity assumptions for the interaction potentials the discrete energy Γ-converges almost surely to a deterministic and homogenous integral functional.

Mathias Schäffner
University of Würzburg (Germany)
mathias.schaeffner@tu-dresden.de

Stefan Neukamm
Technische Universität Dresden
Institute for Scientific Computing
stefan.neukamm@tu-dresden.de

Anja Schlömerkemper
University of Würzburg
anja.schloemerkemper@mathematik.uni-wuerzburg.de

MS34

Molecular Packing Problems and Quotients of the Euclidean Group by Space Groups

Crystallographic space groups are discrete subgroups of the Lie group of Euclidean motions. The configuration spaces of molecular crystals can be viewed as the coset spaces that results from "dividing' the Euclidean group by the space group of the molecular crystal. These spaces appear not to have been studied before. Though flat manifolds and orbifolds are quotients of Euclidean space by crystallographic space groups, and these have been studied, they are not the same as the coset spaces examined here, which are always six-dimensional manifolds. In order to understand these spaces we have had to re-examine the theory of space groups from a new mathematical perspective.

Gregory Chirikjian
Dept. of Mechanical Engineering
Johns Hopkins University
gregc@jhu.edu

MS34

Diffraction and Dynamical Spectra in Aperiodic Order

Diffraction is the main tool to determine order in periodic and aperiodic structures, whereas the dynamical spectrum is a mathematical quantity related to the action of translations on a structure. For mathematical quasicrystals based on a cut and project scheme, the diffraction and dynamical spectra are pure point spectra that are well understood. Indeed, the first proofs of the pure point diffraction property for cut and project sets was based on the connection with the dynamical spectrum, because a pure point dynamical spectrum implies a pure point diffraction spectrum. The situation is more complex for ordered structures with singular continuous or even absolutely continuous diffraction. Examples of such systems can be obtained from (symbolic) substitution rules and their generalisations to higher dimensions. This talk will discuss the relation between diffraction and dynamical spectra for a number of paradigmatic cases, and based on these explain recent general results on the relation between these spectral measures.

Uwe Grimm
Department of Mathematics & Statistics
The Open University
u.g.grimm@open.ac.uk

Michael Baake
Faculty of Mathematics
University of Bielefeld, Germany
mbaake@math.uni-bielefeld.de

MS34

Skeletal Polyhedral Complexes and Nets with High Symmetry

Skeletal polyhedral complexes in ordinary space are geometric edge graphs (nets) equipped with additional polyhedra-like (super) structure determined by the collection of "faces", which can either be simply closed, planar or skew, finite polygons (edge cycles), or zig-zag or helical, infinite polygons (edge paths). We review the present state of the classification of discrete skeletal complexes distinguished by certain transitivity properties of their symmetry groups. Particularly interesting skeletal structures are the regular, chiral, or uniform skeletal polyhedra, as well as more general regular polygonal complexes. These are periodic structures with crystallographic symmetry groups exhibiting fascinating geometric, combinatorial, and algebraic properties, or are finite structures.

Egon Schulte
Department of Mathematics
Northeastern University
schulte@neu.edu

MS34

Comparing Coincidence Rotations and Similarity Transformations of Lattices and Modules

Given a d-dimenional lattice L, the intersection $L \cap RL$ is called a CSL if it is a sublattice of full rank. The set of the corresponding rotations R forms the group $\mathrm{SOC}(L)$. We compare it with the group $\mathrm{SOS}(L)$, comprising all

rotations R arising from similarity transformations λR that map L onto a sublattice of itself. The factor group $\mathrm{SOS}(L)/\mathrm{SOC}(L)$ is Abelian and restricted by the dimension d, with fewer restrictions if we pass on to modules.

Peter Zeiner
Department of Mathematics
University of Bielefeld
pzeiner@math.uni-bielefeld.de

MS35

Isometric Immersions, Energy Minimization and Branch Points in Non-Euclidean Elastic Sheets

The edges of torn elastic sheets and growing leaves often display hierarchical self-similar like buckling patterns. On the one hand, such complex, self similar patterns are usually associated with a competition between two distinct energy scales, e.g. elastic sheets with boundary conditions that preclude the possibility of relieving in plane strains, or at alloy-alloy interfaces between distinct crystal structures. On the other hand, within the non-Euclidean plate theory this complex morphology can be understood as low bending energy isometric immersions of hyperbolic Riemannian metrics. In particular, many growth patterns generate residual in-plane strains which can be entirely relieved by the sheet forming part of a surface of revolution or a helix. In this talk we will show that this complex morphology (i) arises from isometric immersions (ii) is driven by a competition between the two principal curvatures, rather than between bending and stretching. We identify the key role of branch-point (or monkey-saddle) singularities, in complex wrinkling patterns within the class of finite bending energy isometric immersions. Using these defects we will give an explicit construction of strain-free embeddings of hyperbolic surfaces that are fractal like and have lower elastic energy than their smooth counterparts.

John A. Gemmer
Brown University
john_gemmer@brown.edu

Shankar C. Venkataramani
University of Arizona
Department of Mathematics
shankar@math.arizona.edu

Eran Sharon
Racah Institute of Physics
The Hebrew University
erans@mail.huji.ac.il

Toby Shearman
University of Arizona
tshearman@math.arizona.edu

MS35

Metric Frustration Selects Morphology of Chiral Filament Bundles

In this talk, I discuss how geometric frustration selects the morphology of self-twisted filament bundles, an assembly motif critical to biological and synthetic nanomaterials. Uniform inter-filament spacing is incompatible with twist, leading to optimal shapes that break the underlying symmetries of interfilament forces and local packing, paralleling a morphological instability of spherical two-dimensional crystals. Selection of cylindrical vs. tape-like bundle morphology is controlled by the relative costs of filament bending and straining of inter-filament bonds.

Doug M. Hall
Polymer Science and Engineering
University of Massachusetts Amherst
dhall@mail.pse.umass.edu

Isaac R. Bruss
Department of Chemical Engineering
University of Michigan
ibruss@umich.edu

Gregory M. Grason
Polymer Science and Engineering
University of Massachusetts Amherst
grason@mail.pse.umass.edu

MS35

Gaussian Curvature as an Identifier of Shell Rigidity

The rigidity of a shell (for example under compression) is closely related to the optimal Korn's constant in the nonlinear first Korn's inequality for H^1 fields. That constant scales like h^2 for plates with thickness h as shown by Friesecke, James and Mueller, 2002. The situation for shells is less well-understood. One important mathematical question is: How can one compare the rigidity of two different shells? In this talk we classify shells according to their Gaussian curvature and derive sharp Korn's first inequalities for shells with zero, positive and negative Gaussian curvature. This is partially joint work with Yury Grabovsky.

Davit Harutyunyan
University of Utah
davith@math.utah.edu

MS35

Putting Patterns on Pollen

We describe the surface patterning of spherical pollen grains as a first-order phase transition to a spatially modulated phase. The modulated phases occur when some microscopic process has a spatial instability with wavelength λ_0. In the planar case, such as pattern formation on a flat sheet, the preferred ordered state is striped or hexagonal. We show that the ordered states on spheres have a richer phenomenology, and we calculate the states' free energies.

Maxim O. Lavrentovich, Eric Horsley, Asja Radja, Alison Sweeney
Department of Physics
University of Pennsylvania
mlav@sas.upenn.edu, ehorsley@sas.upenn.edu,
asjar@sas.upenn.edu, alisonsw@physics.upenn.edu

Randall Kamien
Physics Dept
University of Pennsylvania
kamien@physics.upenn.edu

MS36

Grain Boundary Character Distribution and Mass

Transport Paradigm

Cellular networks are ubiquitous in nature. Most technologically useful materials arise as polycrystalline microstructures, composed of a myriad of small crystallites or grains, separated by interfaces, or grain boundaries. The energetics and connectivity of the grain boundaries network plays a crucial role in determining the properties of a material across a wide range of scales. The recently discovered grain boundary character distribution (GBCD) is an empirical distribution of the relative length (in 2D) or area (in 3D) of interface with a given lattice misorientation and grain boundary normal. GBCD is a characterization of the texture which is found to be strongly correlated to the interfacial energy. In this talk GBCD is introduced and investigated by the use of a large scale simulations and mathematical analysis. We present the simplified 1D coarsening model of the grain boundary network and discuss an entropy based theory based on mass transport and a Kantorovich-Rubinstein-Wasserstein metric to suggest that, to first approximation, the GBCD behaves like the solution to a Fokker-Planck Equation. The proposed theory is validated numerically and is in agreement with experiments. This is joint work with K. Barmak, P. Bardsley, E. Eggeling, M. Emelianenko, D.Kinderlehrer, R. Sharp and S. Taasan

Yekaterina Epshteyn
Department of mathematics
University of Utah
epshteyn@math.utah.edu

MS36

Kinetic Models for 2D Grain Growth

A fundamental aspect of 2D cellular networks with isotropic line tension is the Mullins-von Neumann $n-6$ rule: the rate of change of the area of a (topological) n-gon is proportional to $n-6$. As a consequence, cells with fewer than 6 sides vanish in finite time, and the network coarsens. Numerical and physical experiments have revealed a form of statistical self-similarity in the long time dynamics. We propose a kinetic description for the evolution of such networks. The ingredients in our model are an elementary N particle system that mimics essential features of the von Neumann rule, and a hydrodynamic limit theorem for population densities when $N \to \infty$. This model is compared with a set of models derived in the physics and materials science communities, as well as extensive numerical simulations by applied mahematicians. This is joint work with Joe Klobusicky (Brown University and Geisinger Health Systems) and Bob Pego (Carnegie Mellon University).

Govind Menon
Brown University
menon@dam.brown.edu

Robert Pego
Carnegie Mellon University
rpego@cmu.edu

Joe Klobusicky
Geisinger Health Systems
joeklob@gmail.com

MS36

Stochastic Processes in Mesoscale Modeling of Polycrystals

This talk summarizes recent analytical results related to self-similarity of grain boundary (GB) distributions during materials coarsening. By adapting continuous time random walk framework, we derive the mesoscopic master equation for GB velocities and prove that it admits a self-similar solution predicted by 1D simulations. This work helps identify stochastic processes governing grain growth, which sheds light on the evolution of other statistics, as well as coarsening rates, dependence on interfacial energy and initial parameters, and is generalizable to higher dimensions.

Diego Torrejon, Maria Emelianenko
George Mason University
diego.torrejon.medina@gmail.com, memelian@gmu.edu

MS36

A New Look on Scaling: The Envelope of Size Distributions in Ostwald Ripening and Grain Growth

The statistical scaling properties of microstructural coarsening by Ostwald ripening and grain growth are studied by means of the envelope of the family of evolving size distribution functions. For any self-similar family of size distributions the envelope is uniquely determined by the growth exponent allowing among others an independent determination of the coarsening parameters without considering individual growth paths. Numerical Potts model studies of grain growth confirm and complement the analytical results.

Dana Zoellner
Otto-von-Guericke University
Magdeburg, Germany
dana.zoellner@ovgu.de

Peter Streitenberger
Otto-von-Guericke University Magdeburg
peter.streitenberger@ovgu.de

MS37

Pair Densities in Density Functional Theory

For a many-electron system, the exact Coulomb repulsive energy is completely determined by the electron pair density, which has not been intensively studied in standard density functional models. We simulate the true pair densities of two groups of one dimensional systems with homogeneous and inhomogeneous single-particle densities, respectively. With the given single-particle densities, we carry out numerical simulations of Hohenberg-Kohn functionals for both bosons and fermions from a strongly interacting limit to a weakly interacting limit.

Huajie Chen
TU Munich
Huajie.Chen@warwick.ac.uk

Gero Friesecke
Centre for Mathematical Sciences
Technische Universität München, Germany

gf@ma.tum.de

MS37

Adaptively Compressed Exchange Operator

The Fock exchange operator plays a central role in modern quantum chemistry, such as in Hartree-Fock calculations and Kohn-Sham density functional theory calculations with hybrid exchange-correlation functionals. We develop the adaptively compressed exchange operator formulation (ACE), which greatly reduces the computational cost associated with the Fock exchange operator without loss of accuracy. The ACE formulation does not depend on the size of the band gap, and thus can be applied to insulating, semiconducting as well as metallic systems. Numerical results indicate that the ACE formulation can become advantageous even for small systems with tens of atoms.

Lin Lin
University of California, Berkeley
Lawrence Berkeley National Laboratory
linlin@math.berkeley.edu

MS37

Tensor Networks and Related Representation for Electronic Schrodinger Equation

Hierarchical Tucker tensor format (Hackbusch) and Tensor Trains (TT) (Tyrtyshnikov) have been introduced recently in numerics offering stable and robust approximation of high order tensors by a low order cost. Considering an occupation number labeling of Slater determinants, the discrete Fock space becomes isometric to $\mathcal{V} = \otimes_{i=1}^{d} \mathbf{C}^2$. Therein these formats are equivalent to tree tensor networks states (TTNS) and matrix product states (MPS) originally introduced for the treatment of quantum lattice systems. For numerical computations, we cast the computation of an approximate ground solution into an optimization problem constraint by the restriction to tensors of prescribed multi-linear ranks $\mathbf{r}$. This optimzation problem can be tackled by alternating directional search or Riemannian optimization methods. The representation described above depends on the choice of the underlying one particle basis. We try to combine orbital rotation with low rank tensor approximation. For the full CI this resembles MSCF calculations, whereas internal rotations often leads to unstabilities.

Reinhold Schneider
Technische Universitat Berlin
schneidr@math.tu-berlin.de

MS37

Spectral Gauss Quadrature Method with Subspace Interpolation for Kohn-Sham Density Functional Theory

Session Code U; Oral; Yes, you can transfer to poster. This talk is on reducing the computational cost of the linear-scaling spectral Gauss quadrature (LSSGQ) method (Suryanarayana et al., JMPS 2013). The LSSGQ method requires a Lanczos procedure at every node in a mesh. We propose a new interpolation scheme, the subspace interpolation that lifts this requirement. Subspace interpolation takes advantage of the overlap in the Krylov-subspaces of neighboring nodes in the mesh. Subspace interpolation performs several orders of magnitude better than a real-space interpolation.

Xin Cindy Wang
U.S. Army Research Laboratory
xin.c.wang2.ctr@mail.mil

MS38

Fundamental Limits to Wave Scattering in Lossy Media

I present new, shape-independent bounds on scattering processes in lossy media, arising only from energy-conservation considerations. I show that the bounds are tight and can be achieved with realistic structures in certain cases, while in others they offer the possibility of orders-of-magnitude improvement over current designs. I briefly discuss the bounds in the context of thermal radiation, where they permit a generalization of the "blackbody" concept to the near field.

Owen D. Miller
Math Dept.
Massachusetts institute of Technology
odmiller@math.mit.edu

MS38

Applications of Herglotz Functions in Poroelastic and Elastic Composite Materials

In this talk, integral representation formula (IRF) for two-phase elastic composite materials will be presented. The implication of the IRF of dynamic permeability functions of poroelastic materials on its approximability by Pronys sum in time-domain will also be addressed.

Yvonne Ou
Associate Professor of Mathematical Sciences
Department of Mathematical Sciences, University of Delaware
mou@udel.edu

MS38

Markov Regularization of Multivariate Moment Sequences of Singular Measures

A. Markov has proposed more than a century ago to solve the moment problem with bounded weights via the imaginary part of the phase of the Cauchy transform of the underlying measure. I will explain how to adapt Markov's idea to several variables and will propose a regularization of moment sequences arising from singular measures supported by convex wedges in Euclidean space. An application to the spectral analysis of the Koopman operator of certain chaotic dynamical systems will be sketched.

Mihai Putinar
Professor of Mathematics
Newcastle University, Newcastle upon Tyne, UK
mihai.putinar@ncl.ac.uk

MS39

Efficient and Robust Free Energy Calculations in Materials

Methods for calculating the free energy, which describes a system's equilibrium behavior, can be based on the the system's probability density or on expectation values of forces.

We have developed a method for free-energy surface exploration and reconstruction that combines aspects of several methods with Gaussian process regression to reduce computational cost. We use a harmonic potential model system to understand the relation between probability-density-based and force-based free energy reconstructions.

Noam Bernstein
Naval Research Laboratory
noam.bernstein@nrl.navy.mil

MS39

From Atomistic to Systematic Coarse-Grained Models for Molecular Systems

Here we give an overview of different methods for obtaining optimal parametrized coarse-grained models, starting from detailed atomistic representation for high dimensional molecular systems. Methods such as inverse Monte Carlo, inverse Boltzmann, force matching, relative entropy, provide parameterizations of coarse-grained models at equilibrium by minimizing a fitting functional over a parameter space. We further extend these studies using path-space methods (relative entropy rate) for coarse-graining and uncertainty quantification for non-equilibrium processes.

Vagelis Harmandaris
University of Crete
harman@uoc.gr

Evangelia Kalligiannaki
University of Southern California
vageliwka@gmail.com

Markos A. Katsoulakis
University of Massachusetts, Amherst
Dept of Mathematics and Statistics
markos@math.umass.edu

Petr Plechac
University of Delaware
Department of Mathematical Sciences
plechac@math.udel.edu

MS39

Surface Hopping Algorithms for Mixed Quantum-Classical Dynamics

Surface hopping algorithm is widely used in chemistry for mixed quantum-classical dynamics, while it is not yet clear whether it can be derived asymptotically. We will discuss some recent progress in semiclassical asymptotics and understanding for the surface hopping algorithms.

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

MS39

Modeling the Mechanics of 2D Layered Heterostructures

The synthesis of graphene, a one-atom thick 2D graphitic sheet, was a revolution in materials physics. Since then a host of other 2D materials have been discovered that can be stacked to create layered heterostructures with remarkable properties. Due to the weak van der Waals interaction between layers, the resulting structures can be incommensurate and therefore challenging to model. We describe recent work on developing a computational method for modeling the mechanics of 2D heterostructures.

Ellad B. Tadmor
Department of Aerospace Engineering & Mechanics
University of Minnesota
tadmor@aem.umn.edu

MS40

The Mechanics of Gap Formation in Endothelial Cell Monolayers

The formation of gaps in human endothelial cell monolayers leads to fatal illness. A computer model on an amorphous assembly of adhesive particles, subjected to an imposed tension has been developed to gain microscopic understanding of gap formation. Molecular Dynamics simulations of this model show a rate-of-tension dependent transition; at high rates the monolayer moves from an elastic to a "plastic' regime. This second regime, where pre-existing gaps increase in size associated to long range stress correlations, bears intriguing similarities with the experimental finding.

Joyjit Chattoraj, Emanuela Del Gado
Georgetown University
Department of Physics
Joyjit.Chattoraj@georgetown.edu,
emanuela.del.gado@georgetown.edu

C. Corey Hardin
Massachusetts General Hospital, Boston, MA
Division of Pulmonary and Critical Care Medicine
chardin@partners.org

Ramaswamy Krishnan
Beth Israel Deaconess Medical Center, Boston, MA
Center for Vascular Biology Research
rkrishn2@bidmc.harvard.edu

MS40

Crack Propagation in Bone: The Role of Sacrificial Bonds

The glue at the interface between mineralized collagen fibrils is hypothesized to play an essential role in retaining the integrity of bone structure at the microscale. The glue is a disordered non-collageneous protein that evolved a mechanism for creating more entropy -if needed- with increased deformation through the sacrificial bonds and hidden length system. The manipulation of entropy and state of disorder enables the polymer to dissipate more energy upon stretching leading to tougher mineralized collagen fibril assembly. I will present a statistical thermodynamics model integrating the wormlike chain model, the transition state theory and fracture mechanics that examines the rate and displacement response of the glue phase and its implications on the fracture response of the collagen fibrils.

Ahmed Elbanna
Department of Civil and Environmental Engineering
University of Illinois, Urbana-Champaign

elbanna2@illinois.edu

MS40

Elastic Free Energy and the Shapes of Growing Tumors

It is well established that the mechanical environment influences cell functions in health and disease. In this talk, we will address how the mechanical environment influences tumor growth, in particular, the shape of solid tumors. In an in vitro tumor model, which isolates mechanical interactions between cancer tumor cells and a hydrogel, we have found that tumors grow as ellipsoids, resembling the same, oft-reported observation of in vivo tumors. Specifically, an oblate ellipsoidal tumor shape robustly occurred when the tumors were grown in hydrogels that were stiffer than the tumors, but when they were grown in more compliant hydrogels they remained closer to spherical in shape. Using large scale, nonlinear elasticity computations we showed that the oblate ellipsoidal shape minimizes the elastic free energy of the tumor-hydrogel system. Having eliminated a number of other candidate explanations, we hypothesized that minimization of the elastic free energy is the reason for predominance of the experimentally observed ellipsoidal shape. Such studies result may hold significance for explaining the shape progression of early solid tumors in vivo and could be an important step in understanding the processes underlying solid tumor growth.

Krishna Garikipati
Mechanical Engineering
University of Michigan
krishna@engin.umich.edu

Kristen Mills
Rensselaer Polytechnic Institute
millsk2@rpi.edu

Shiva Rudraraju
University of Michigan
rudraa@umich.edu

Ralf Kemkemer
Universitaat Reutlingen
ralf.kemkemer@reutlingen-university.de

MS40

Motility Driven Glass Transitions in Biological Tissues

Biological tissues involved in important functions such as wound healing, embryonic development, and cancer tumorigenesis have recently been shown to be close to a glass or jamming transition. However, existing particle-based theories can not explain observations of jamming transitions in confluent biological tissues, where there are no gaps between cells and the packing fraction is always unity. I will discuss our new theoretical framework for predicting energy barriers and rates of cell migration in confluent tissue monolayers, and show that this model predicts a novel type of jamming transition, which takes place at constant packing fraction and depends only on single cell properties such as cell-cell adhesion, cortical tension and persistent active cell motility. I will show that our a priori theoretical predictions are precisely realized in cell cultures from human patients with implications for asthma pathobiology, and discuss how these ideas might also be applied to understand the epithelial-to-mesenchymal transition and cancer tumor metastasis.

Lisa Manning
Department of Physics
Syracuse University
mmanning@syr.edu

MS41

Modeling Dynamics of Mucous Flows

Mucus rheology is tuned across the human body to protect every organ. We focus this lecture on lung mucus which, when "healthy", traps and clears billions of inhaled particulates and pathogens every day. Experiments and data to assess both diffusive and flow transport properties will be presented along with the current status of our modeling effort.

M. Gregory Forest
University of North Carolina at Chapel Hill
Dept of Math & Biomedical Engr.
forest@unc.edu

Paula A. Vasquez
University of South Carolina
paula@math.sc.edu

MS41

Transport of Charged Particles in Biological Environments.

Abstract not available

Chun Liu
Department of Mathematics, Penn State University
University Park, PA 16802
liu@math.psu.edu

MS41

Stochastic and Multi-Scale Dynamics of Stem Cells and Developmental Patterning.

Noise and stochastic effect play important roles at all scales in complex biological systems. In this talk, I will discuss strategies and principles for noise attenuation and robustness to genetic and environmental perturbations in signal transduction, embryonic patterning, and regeneration driven by stem cells. In one case, I will introduce a critical quantity that dictates capability of attenuating temporal noise in feedback systems. In another case, I will show that noise in gene regulations actually enables reduction of stochastic effects in spatial patterns during embryonic development. Finally, novel experimental data that support our modeling and computational predictions will be presented and several multi-scale, stochastic, and computational modeling frameworks that are required for simulating such complex biological systems will be introduced.

Qin Nie
Department of Mathematics
U. of California at Irvine
qnie@math.uci.edu

MS41

Biological Plywoods

This lecture presents analysis and simulation of the self-assembly, fiber structure, and functionality of biological

plywoods, as found in plant cell walls, the cuticle of bettles, and in biomimetic processing of collagen solutions. The formation of the cholesteric Bouligand structure by directed chiral self-assembly and generation of cellular patterns is characterized with respect to rotational diffusivity, anchoring, diffusionless growth. Geometric modelling of ideal and non-ideal plywoods is effected and validated for cornea-like and graded plywoods. Finally, nanowrinkling in plywoods is explained and characterized using chiral capillarity and chiral shape equations. The resulting optical properties of nano-wrinkled surfaces is compared to irrident colours in flowers.

Alejandro D. Rey
Department of Chemical Engineering
McGill University
alejandro.rey@mcgill.ca

MS42

Coarse-Graining from Atomistic to Continuum Models for Island and Step Dynamics during Epitaxial Growth and Relaxation

Challenges remain for coarse-graining of atomistic lattice-gas models for epitaxial growth and relaxation to BCF-type continuum step dynamics models. Reliable determination of the kinetic coefficients and permeability controlling step dynamics is key. Such coefficients when incorporated into step dynamics modeling should precisely recover behavior of the atomistic models, a feature not always achieved using traditional expressions. We present a new approach based on analysis of discrete 2D deposition-diffusion equations in geometries incorporating step edge structure.

James Evans
Ames LaboratoryUSDOE
Dep of Physics & Astro and Dep of Math, Iowa State Univ
evans@ameslab.gov

MS42

Island Dynamics Model for Mound Formation: Effect of a Step-Edge Barrier

We have developed an island dynamics model for epitaxial growth with the level-set technique, where islands are treated as continuous in the x-y-plane, while individual atomic layers are resolved in the z-direction. Adatoms are treated as a mean field quantity by solving a diffusion equation. We will discuss an analytic derivation for the proper expression for the equilibrium adatom density at the step edge in the presence of a step-edge barrier. The effect of an additional step-edge barrier is incorporated via a mixed Robin-type boundary condition for the diffusion equation. We will present a numerical scheme to solve such a boundary condition on a fixed grid with moving boundaries. We will show how the inclusion of the step-edge barrier leads to the formation of mounds that become progressively steeper as the step-edge barrier increases. Finally, we will discuss how we can include the effect of downward funneling in our model, and how it leads to the stabilization of the slope of the mounds.

Christian Ratsch
UCLA
Department of Mathematics
cratsch@math.ucla.edu

MS42

Epitaxial Growth of Graphene

Using the multimode phase field crystal model [Mkhonta et al, Phys. Rev. Lett. 111 (2013) 035501] in combination with the vapor phase approach [Schwalbach et al, Phys. Rev. E 88 (2013) 023306] allows to model epitaxial growth of crystals with a honeycomb structure (graphene). We use this approach and study the influence of a hexagonal substrate (Cu foil) on nucleation, growth morphology and defect formation.

Axel Voigt
TU Dresden
axel.voigt@tu-dresden.de

MS43

Hydrodynamic Limit of a KMC Model for a Layered Cake Structure and Facet Formation

Abstract not available

Hala A.H. Shehadeh
James Madison University
alhajjhy@jmu.edu

MS43

Modeling Effect of Flow on Crystallization Kinetics: From Kinetic Theory to Hydrodynamics

Equilibrium theory of solid-liquid phase transitions is well understood. The non-equilibrium theory for phase transitions is however not well developed. This talk will outline a general approach of building a time dependent hydrodynamic theory for phase transition from a kinetic theory. This coarse-graining approach leads to a meso-scale time dependent theory that is shown to be a time dependent density functional theory of freezing. The model is applied to study the effect of flow on solid liquid phase transitions.

Arvind Baskaran
University of California, Irvine
baskaran@math.uci.edu

Aparna Baskaran
Brandeis University
Department of Physics
aparna@brandeis.edu

John Lowengrub
Department of Mathematics
University of California at Irvine
lowengrb@math.uci.edu

MS43

On the Connection Between Kinetic Monte Carlo and Burton-Cabrera-Frank Theory of Step-Flow in 1+1 Dimensions

The Burton-Cabrera-Frank (BCF) theory of step flow is regarded as a valuable model for describing nanoscale evolution of crystal surfaces. In this talk, I discuss a formal derivation of a single-step, BCF-type model from a discrete master-equation model of a crystal surface in 1+1 dimen-

sions without external deposition. The key steps of the derivation amount to (I) formulating the discrete model in such a way that the step position is a measurable property of the system, and (ii) defining quantities of the BCF theory in terms of appropriate averages taken over the discrete states. Importantly, the analysis also relies on the observation that the number of adatoms on a surface is typically small at experimentally relevant temperatures. Mathematically, this fact is expressed via a maximum principle, which we invoke in coordination with appropriate initial conditions to control corrections to the BCF model. As a result, the derivation (i) provides a mathematical interpretation for how the BCF model is a near-equilibrium theory, and (ii) reveals the atomistic origins of its underlying material parameters.

Paul Patrone
Department of Physics, University of Maryland, College Park
NIST Gaithersburg
paul.patrone@nist.gov

MS43

Peridynamic Models for Upscaling Crystalline Structures

Session code: AR; Oral; No, transfer to poster. Peridynamics is a nonlocal reformulation of classical continuum mechanics, based on integral equations. Classical atomistic models are also nonlocal and account for long-range interactions. There exists a similarity between the computational structure of discretized peridynamic equations and molecular dynamics. In this talk, we will demonstrate that peridynamic models can be cast as upscaled atomistic models for crystalline structures, providing means for simulating atomistic systems at a greatly reduced computational cost. Analytical comparisons of equations of motion and dispersion relations will be presented along with supporting computational results.

Pablo Seleson
Oak Ridge National Laboratory
selesonpd@ornl.gov

MS44

Homogenization of Composite Ferromagnetic Materials

Nowadays, nonhomogeneous and periodic ferromagnetic materials are the subject of a growing interest. Actually such periodic configurations often combine the attributes of the constituent materials, while sometimes, their properties can be strikingly different from the properties of the different constituents. In this talk, after a brief review of some basic ideas in homogenization theory (De Giorgi's notion of Γ-convergence and Nguetseng-Allaire notion of two-scale convergence, I will introduce the micromagnetic model of magnetized matter. In this framework I will present the results of a recent work concerning the rigorous derivation of the homogenized Gibbs-Landau free energy functional associated to a composite periodic ferromagnetic material, i.e. a ferromagnetic material in which the heterogeneities are periodically distributed inside the media. I thus describe the Γ-limit of the Gibbs-Landau free energy functional, as the period over which the heterogeneities are distributed inside the ferromagnetic body shrinks to zero.

Francois Alouges
University of Paris-Sud, Orsay
Francois.Alouges@math.u-psud.fr

Giovanni Di Fratta
Ecole Polytechnique, Paris
difratta@cmap.polytechnique.fr

MS44

A Mean-Field Model for Spin Dynamics in Multilayered Ferromagnetic Media

Magnetic storage devices rely on the fact that ferromagnetic materials are typically bistable, and that it is possible to switch between different states by applying a magnetic field. The discovery of Giant Magneto-Resistance effect has enabled the use of layered ferromagnetic materials in magnetic devices, such as magnetic memories (MRAMs). Even in the absence of thermal effects, there are limitations in the storage capacity of such devices due to the fact that as the size is decreased, the magnitude of the switching field increases due to an increase in shape anisotropy. Given that magnetic fields have long range, the density of such devices is limited. A new mechanism for magnetization reversal in multilayers was proposed by Slonczweski and Berger, whereby an electric current flows perpendicular to the layers. The current is polarized in the first layer, and the polarization travels with the current to the second layer, where it interacts with the underlying magnetization. Since currents are localized in each cell, long range effects can be reduced. In this talk we will discuss the connection between several models for the description of the spin transfer torque at different physical scales. Specifically, we connect the quantum and kinetic descriptions with the help of Wigner transform, and the kinetic and diffusion models by a specific parabolic scaling. Numerical examples will be presented to illustrate the applicability and limit of the different models.

Jingrun Chen
University of California, Santa Barbara
cjr@math.ucsb.edu

Carlos Garcia-Cervera
Mathematics, UCSB
cgarcia@math.ucsb.edu

Xu Yang
Department of Mathematics
University of California, Santa Barbara
xuyang@math.ucsb.edu

MS44

Current Induced Torques in Magnetic Thin Films and Devices: Physics and Modeling

The magnetization of a magnetic material can be reversed by using electric currents that transport spin angular momentum. In the reciprocal process a changing magnetization orientation produces currents that transport spin angular momentum. Understanding how these processes occur reveals the intricate connection between magnetization and spin transport, and can transform technologies that generate, store or process information via the magnetization direction. In this talk I will explain how currents can generate torques that affect the magnetic orientation in a variety of magnetic materials and sample geometries. Modeling the magnetization dynamics is challenging principally because current induced torques are generally non-

conservative and thus cannot be described in terms of a gradient of an effective energy. Further, noise induced processes (usually thermal fluctuations) typically need to be considered. There is, however, intense interest and efforts to model both long-time dynamics (rare events triggered or assisted by spin-torques) and short-time dynamics, where spin-transfer torques drive dynamics that occurs on subnanosecond time scales (the natural time scale of magnetization dynamics in ferromagnetic materials). I will present examples of experiments in my group on current induced magnetization switching and precession and present models we have explored of spin-transfer torque driven dynamics in the presence of thermal noise.

Andrew Kent
NYU, Department of Physics
adk1@nyu.edu

MS44

Magnetic Domains in Thin Ferromagnetic Films with Strong Perpendicular Anisotropy

We consider a regime of large and ultra-thin ferromagnetic films with strong anisotropy and easy axis pointing out of the film plane. Starting from the full three-dimensional micromagnetic model, we identify (to leading order) the critical scaling where the phase transition from single domain states to multi-domain states such as bubble or maze patterns occurs. Furthermore, we derive the asymptotic behavior of the energy in the single domain regime within the framework of Γ-convergence.

Hans Knuepfer
University of Heidelberg
knuepfer@uni-heidelberg.de

Cyrill B. Muratov
New Jersey Institute of Technology
Department of Mathematical Sciences
muratov@njit.edu

Florian Nolte
University of Heidelberg
Institute for Applied Mathematics
f.nolte@uni-heidelberg.de

MS45

Superlensing Using Hyperbolic Metamaterials

We consider the diffusion or the Helmholtz equations in a bounded domain, which contains a sub-region D made of a medium, whose coefficients have a non-elliptic real part, and a small imaginary part of size δ. We are particularly interested in the case when the real part of the metamaterial leads to a hyperbolic PDE in D when $\delta = 0$. We exhibit material parameters, geometries and source terms for which superlensing takes place as $\delta \to 0$.

Eric Bonnetier
Université Joseph Fourier, Grenoble
Laboratoire Jean Kuntzmann
eric.bonnetier@imag.fr

Hoai-Minh Nguyen
École Polytechnique Fédérale de Lausanne
hoai-minh.nguyen@epfl.ch

MS45

A Three-Sphere Inequality and Cloaking Using Complementary Media in the Finite Frequency Regime

Motivated from cloaking using complementary media in the finite frequency regime, we establish a three sphere inequality for second order elliptic equations with respect to Cauchy data. The proof follows from the unique continuation principle due to a very beautiful result of M.H. Protter in 1960. This three sphere inequality, together with the technique of removing localized singularity introduced by H.M. Nguyen, can be used to prove a cloaking result in the finite frequency regime. In particular, no smallness condition for the cloaked region is required as the frequency is large. This is a joint work with Hoai-Minh Nguyen.

Loc Nguyen
UNC Charlotte
lnguye50@uncc.edu

MS45

ALR with Maxwell's Equations

We consider electromagnetic scattering from a layered metamaterial in $\mathbf{R}^3$ with a fixed positive frequency. First we show that in the case of nonmagnetic media there is no analogue of ALR. Secondly, we give examples of weak anomalous resonance for doubly negative media, and consider criteria for non-existence also in this case. Finally we study the quasi static limit of Maxwell's equations and try to understand the possible appearance of resonances on the limit. Also, if time permits, we consider what happens for a dielectric inclusion in the presence of a negative material layer.

Petri Ola
University of Helsinki
petri.ola@helsinki.fi

Matti Lassas
University of Helsinko
matti.lassas@helsinki.fi

MS45

Uniform Refraction in Negative Refractive Index Materials

Session code: X; oral; yes, you can transfer to poster. We study the problem of constructing an optical surface separating two isotropic media, one of which has a negative refractive index. We develop a vector form of Snell's law, which is used to study surfaces possessing a certain uniform refraction property, both in the near and far field. In the near field problem, unlike the case when both materials have positive refractive index, we show that the resulting surfaces can be neither convex nor concave.

Eric Stachura
Temple University
eric.stachura@temple.edu

Cristian Gutierrez
Department of Mathematics
Temple University

gutierre@temple.edu

MS46

Nonlinear Quantum Mechanics

We model the dynamics of electrons in doped quantum wells driven by terahertz radiation and a superlattice biased by a dc voltage. We compute coherent, self-consistent electron states, density matrix equations of motion, and dipole absorption spectra. The model simultaneously accounts for intersubband transitions and many nonlinear phenomena that have been observed in these systems. We predict a bistable response for strong terahertz fields and bifurcations to coherent time-periodic quantum states. These bifurcation include, period-doubling bifurcations, producing a subharmonic response, Hopf bifurcations producing an incommensurate frequency response, and a cascade of period doubling bifurcations to a strange attractor. We also see a cascade of quasi-periodic orbits on the Hopf torus to a strange attractor. These bifurcation have been difficult to measure in single quantum wells. Therefore we design super-lattice heterostructures of quantum wells where these bifurcations occur and are easier to measure.

Bjorn Birnir
University of California Santa Barbara
Department of Mathematics
birnir@math.ucsb.edu

MS46

Modeling Rare Events

Many important dynamic processes in nature can be viewed as being rare events. They don't occur very often but if they do occur, they have drastic consequences. We will discuss the mathematical framework for describing such events, as well as the numerical algorithms that have been developed. We will discuss applications to problems that arise in material science.

Weinan E
Princeton Univesity
Department of Mathematics
weinan@math.princeton.edu

MS46

Euler Sprays and Optimal Transportation

We describe a connection between Arnold's least-action principle for the Euler equations and Wasserstein distance. A relation with Brenier's notion of generalized Euler flows and Peter Smereka's kinetic model for turbulent Euler flows will be sketched.

Robert Pego
Carnegie Mellon University
rpego@cmu.edu

Jian-Guo Liu
Duke University
jian-guo.liu@duke.edu

Dejan Slepcev
Carnegie Mellon University
slepcev@math.cmu.edu

MS47

Dynamics of Polycrystalline Networks

This study is focused on a topological/geometrical representation of polycrystalline networks to obtain statistical predictions of the grain size and face number distributions, including growth 'trajectories' during steady state grain growth. Polyhedral boundaries, triple junctions, and quadruple points are the geometrically distinct network elements that can be rate limiting during grain growth. Evolution of polycrystalline networks exhibit kinetic behavior that entail several kinetic mechanisms through which the required decrease in network energy occurs.

Martin E. Glicksman
Florida Institute of Technology
mglicksman@fit.edu

Paulo Rios
Escola de Engenharia Industrial
prrios@id.uff.br

MS47

Thin Film Deposition Using Rarefied Gas Jet

The rarefied gas jet of Aluminium is studied at Mach number $Ma = (U_j/\sqrt{kbT_j/m})$ in the range $0.01 < Ma < 2$, and Knudsen number $Kn = (1/(\sqrt{2}\pi d^2 n_d H)$ in the range $0.01 < Kn < 15$, using two-dimensional (2D) Direct Simulation Monte Carlo (DSMC) simulations, to understand the flow phenomena and deposition mechanisms in a physical vapor deposition (PVD) process. Here, H is the characteristic dimension, U_j and T_j are the jet velocity and temperature, n_d is the number density of the jet, d is the molecular diameter and kb is the Boltzmann constant.The variation of the local fluxes along the streamwise direction away from the jet are studied. The qualitative nature of the local flux at high Mach number ($Ma = 2$) is similar to those in the incompressible limit ($Ma = 0.01$). These include the initial fast decay, then slow variation, and finally rapid decay near the substrate. However, there are important differences. The amplitudes of the local flux increase as the Mach number increases. An important finding is that the capture width (cross-section of the gas jet deposited on the substrate) is symmetric around the centerline of the substrate, and decreases with increased Mach number due to an increase in the momentum of the gas molecules.

Dr. Sahadev Pradhan
Department of Chemical Engineering
Indian Institute of Science, Bangalore- 560012, India.
sahadevpradhan2015@gmail.com

MS47

Phase Field Models of Creep in Polycrystals

In this talk I will review the recently developed phase field model of diffusional creep, and explore discuss simulations of this model in one and two dimensions. In addition to capturing a range of physical phenomena in a compact form, the model points the way towards robust descriptions of materials behavior where vacancies play a decisive role in the dynamics. In addition to discussing the advantages of the model, a discussion of the numerous assumptions at the heart of this approach will be detailed, as well as some of the surprises that result from a naive inclusion of

interface energy anisotropy.

James Warren
National Institute of Standards and Technology
Materials Science and Engineering Laboratory
jwarren@nist.gov

Arvind Baskaran
Materials Science and Engineering Division
Material Measurement Lab, NIST
arvind.baskaran@nist.gov

MS48

Ab-initio Dynamics from Electronic to Molecular Scales

Many interesting physical and chemical phenomena require modeling of electronic excited states. We present a methodology based on time-dependent density functional theory for electrons, and classical (Ehrenfest) dynamics for the ions, that allows efficient time propagation of large systems (up to ~ 1000 atoms) for time scales of order 10^{-12} sec. Our method allows the realistic modeling of processes like chemical reactions at surfaces and charge transfer in organic-inorganic interfaces related to photovoltaic applications.

Efthimios Kaxiras
Dept. of Physics and School of Engg. and Applied Sciences
Harvard University
kaxiras@physics.harvard.edu

MS48

Multiscale Modeling and Computation of Optically Manipulated Nano Devices

We present a multiscale modeling and computational scheme for optical- mechanical responses of nanostructures. The multi-physical nature of the problem is a result of the interaction between the electromagnetic (EM) field, the molecular motion, and the electronic excitation. To balance accuracy and complexity, we adopt the semi-classical approach that the EM field is described classically by the Maxwell equations, and the charged particles follow the Schr oidnger equations quantum mechanically. To overcome the numerical challenge of solving the high dimensional multi-component many- body Schr odinger equations, we further simplify the model with the Ehrenfest molecular dynamics to determine the motion of the nuclei, and use the Time- Dependent Current Density Functional Theory (TD-CDFT) to calculate the excitation of the electrons. This leads to a system of coupled equations that computes the electromagnetic field, the nuclear positions, and the electronic current and charge densities simultaneously. In the regime of linear responses, the resonant frequencies initiating the out-of-equilibrium optical-mechanical responses can be formulated as an eigenvalue problem. A self-consistent multiscale method is designed to deal with the well separated space scales. The isomerization of Azobenzene is presented as a numerical example.

Di Liu
Michigan State University
Department of Mathematics
richardl@math.msu.edu

MS48

Correlated Methods for Periodic Systems Based on Localized Resolution of Identity Technique

We describe an atomic-orbital based implementation of correlated methods for periodic systems, making use of the localized resolution of identity technique. By correlated methods, we mean approaches that require information of unoccupied states, such as random-phase approximation and the GW approximation. These will be taken as examples to demonstrate the algorithm as well as the accuracy and efficiency of our implementation in the FHI-aims code.

Xinguo Ren
University of Science and Technology of China
renxg@ustc.edu.cn

MS49

Collective Dynamics on Large Scales - A Phase Field Crystal Like Approach

Abstract not available

Francesco Alaimo
TU Dresden
francesco.alaimo@tu-dresden.de

MS49

Collisions of Deformable Cells Lead to Collective Migration

Abstract not available

Igor S. Aronson
Argonne National Laboratory
aronson@anl.gov

MS49

Modelling the Cell Cytoskeleton as an Active Polar Gel: Cell Deformation and Movement

Abstract not available

Rhoda Hawkins
University of Sheffield
rhoda.hawkins@physics.org

MS49

Collective Motion of Cells under the Influence of Hydrodynamics

Abstract not available

Axel Voigt
TU Dresden
axel.voigt@tu-dresden.de

MS50

Overcoming Bad Scaling Using Ensemble Samplers

In this talk I will discuss a family of ensemble sampling schemes for overcoming timescale separations in badly scaled canonical sampling problems. Typically the usable timestep in molecular dynamics simulations is governed by

the fastest degrees of freedom in the system. Our proposed schemes utilize local scaling information from parallel replicas to speed up the slower motions of the system, without adding significant computational overhead or numerical bias.

Charles Matthews
University of Chicago
c.matthews@uchicago.edu

Ben Leimkuhler
University of Edinburgh
School of Mathematics
b.leimkuhler@ed.ac.uk

Jonathan Weare
University of Chicago
Department of Statistics and the James Franck Institute
weare@uchicago.edu

MS50

Accelerated Sampling of Exit Rates for Molecular Dynamics Using a Homotopy Approach

We developed a new method for approximating exit rates for molecular dynamics with metastable regions. To accelerate the sampling we create several smoothed potentials from the original one in which the exit rate is way easier to sample. For this we introduce a new parameter λ into the potential which control the smoothing. We try to connect the λ to the exit rate to use this dependency to approximate the real exit rate.

Marcus Weber
Zuse Institute Berlin (ZIB)
weber@zib.de

Jannes Quer
Zuse Institute Berlin
quer@zib.de

MS50

Error Estimates for Transport Coefficients in Molecular Dynamics

I present error estimates for transport coefficients, which can be obtained either by the linear response of appropriately perturbed stochastic dynamics, or, equivalently, through the time integration of correlation functions. I consider two issues: the reduction of the bias arising from the numerical integration of continuous dynamics (typically, Langevin dynamics integrated with splitting schemes), and the reduction of the variance through appropriate variance reduction techniques for nonequilibrium systems.

Gabriel Stoltz
ENPC, Paris
gabriel.stoltz@enpc.fr

MS50

Optimal Control of Multiscale Systems Using Reduced-Order Models

We study the asymptotic limit of certain optimal control problem in multiscale stochastic dynamics. By relating the optimal control problem to certain exponential type expectation of the uncontrolled dynamics and adopting the asymptotic analysis method, we formally show that in the time-scale seperation limit, the value function of the optimal control problem for multiscale dynamics converges to its counterpart for the reduced dynamics. We estimate the error bound on the cost function by the uniform error bound on the control policy. With these estimates, we construct the control policy for the multiscale dynamics by studying the reduced dynamics and conclude that the cost function acheives optimality asymptotically. Typical examples are studied.

Wei Zhang
Free University of Berlin
wei.zhang@fu-berlin.de

Carsten Hartmann
FU Berlin
chartman@mi.fu-berlin.de

Juan Cristobal Latorre
Free university of Berlin
jcbiagini@gmail.com

Grigorios Pavliotis
Imperial College London
gpavliotis@gmail.com

MS51

Propagation of Complex Fracture Using Nonlocal Cohesive Forces

We report on a nonlocal cohesive model of peridynamic type for calculating free fracture patterns inside a cracking body. We identify a process zone characterized by strong nonlinearity and dynamic instability. This zone is found to concentrate on a set of zero volume in the limit of vanishing non-locality. $\Gamma-$convergence methods show that the limit dynamics has bounded Griffith surface energy and is elastodynamic away from the fracture set. This approach also is used to identify limits of dynamics associated with phase field methods.

Robert P. Lipton
Department of Mathematics
Louisiana State University
lipton@math.lsu.edu

MS51

On the Variational Convergence of a Class of Nonlocal Functionals Related to Peridynamics

We present a recent study of a variational problem involving a class of nonlocal elastic energies of peridynamic-type on a bounded domain. The associated equilibrium equation is a nonlinear system of coupled integral equations. The well posedness of the variational problem is established via a careful study of the associated energy space. In the event of vanishing nonlocality, the variational convergence of the nonlocal energy to a corresponding classical energy is established. We will also discuss an L^p-compactness result (valid on bounded domain), based on near-boundary estimates, that is used to study the variational limit of minimization problems subject to various volumetric constraints. For energy functionals in suitable form, we find the corresponding limiting energy explicitly. As a special case, the classical Navier-Lamé potential energy is realized as a limit of linearized peridynamic energy, offering a rigorous connection between the nonlocal peridynamic model to classical mechanics for small uniform strain. This is a

joint work with Qiang Du of Columbia University.

Tadele Mengesha
University of Tennessee
mengesha@utk.edu

MS51

On the Consistency Between Nearest-Neighbor Peridynamics and Finite Difference Classical Elasticity

The peridynamics theory of solid mechanics is a nonlocal reformulation of the classical theory of continuum mechanics. It has been demonstrated that, at the continuum level, governing peridynamic equations reduce to classical (local) equations in the limit of vanishing nonlocality, for smooth deformations. Such connection has not been extensively explored, however, at the discrete level. For code verification purposes, it is common practice to solve peridynamic problems with nearest-neighbor discretizations in an attempt to recover classical solutions. In this talk, we will discuss the consistency between nearest-neighbor discretizations of linear elastic peridynamic models and finite difference discretizations of the Navier-Cauchy equation of classical elasticity. We will demonstrate that for those discretizations, standard meshfree methods in peridynamics do not reduce, in general, to corresponding discretized classical models. We will present nodal-based quadratures in peridynamics and derive quadrature weights that give the desired consistency. Results will be presented for one-dimensional bond-based and two dimensional state-based peridynamic models.

Pablo Seleson
Oak Ridge National Laboratory
selesonpd@ornl.gov

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

Michael L. Parks
Sandia National Laboratories
mlparks@sandia.gov

MS51

Numerical Approximations for Two-Dimensional Nonlocal Phase-Field Crystal Models by Fourier Spectral Methods

Session Code: K; oral; Yes, can transfer to poster A nonlocal phase-field crystal (NPFC) model is proposed analogously to the local phase-field crystal (LPFC) model. It is proved that Fourier spectral methods are asymptotically compatible for two-dimensional nonlocal diffusion equations. We further show that Fourier spectral methods are also asymptotically compatible with convergence rate $O(\delta^2)$ for the two-dimensional time-dependent nonlinear NPFC model. On the other hand, a hybrid algorithm by combining truncated series expression and Runge-Kutta method is developed to compute eigenvalues to nonlocal operators. Numerically, it is shown that this hybrid algorithm is robust, efficient and accurate. Simulations demonstrate that NPFC models with sign changing kernels can produce some different interesting periodic crystal structures comparing to local models.

Jiang Yang
Columbia University
jyanghkbu@gmail.com

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

MS52

Computational Model of Substrate-Based Cell Motility

Cell motility and collective migration are among the most important themes in cell biology, mathematical biology, and bioengineering. We propose a computational model based on the phase field method, which is especially suited to treat the moving and deformable boundaries involved in cell motility. We investigate how cells navigate on substrates with patterned adhesion properties and modulated stiffness. For multiple cells, the model predicts that collective cell migration emerges spontaneously as a result of inelastic collision-type interactions of cells.

Igor S. Aronson
Argonne National Laboratory
aronson@anl.gov

MS52

Active Liquid Crystal Models and Applications to Complex Biological Systems

We present a general framework for deriving hydrodynamic models for active liquid crystal systems. We then analyze the mathematical properties of a simplified model and study the spatial-temporal patterns the model predicts subject to physical boundary conditions. Then, we will apply to model to study cell motility and mitosis.

Qi Wang
University of South Carolina
Beijing Computational Science Research Center
qwang@math.sc.edu

Jia Zhao
University of south Carolina
zhao62@math.sc.edu

Xiaogang Yang
Beijing Computational Science Research Center
yangxiaogang@csrc.ac.cn

MS52

A Multiphasic Complex Fluids Model for Cytokinesis of Eukaryotes

Cell Mitosis is a fundamental process in eukaryotic cell reproduction, during which parent cells nucleus first dissembles leading to DNA and chromosome replication, then chromosomes migrate to new locations within the parent cell to form offspring nuclei which triggers cytokinesis leading to the formation of two offspring cells eventually. In this presentation, we develop a full 3D multiphase hydrodynamic model to study the fundamental mitotic mechanism in cytokinesis, the final stage of mitosis. The model describes the cortical layer, a cytoplasmic layer next to the cell membrane rich in F-actins and myosins, as an active liquid crystal system and integrate the extra cellular matrix material and the nucleus into a multiphase complex

fluid mixture. With the novel active matter model built in the system, our 3D simulations show very good qualitative agreement with the experimental obtained images. The hydrodynamical model together with the GPU-based numerical solver provides an effective tool for studying cell mitosis theoretically and computationally.

Jia Zhao
University of South Carolina
zhao62@mailbox.sc.edu

MS52

Nonlinearities and Symmetry Breaking in Active Biological Matter

Abstract not available

Tanniemola liverpool
University of Bristol
t.liverpool@bristol.ac.uk

MS53

Kinetic Models for Crystalline Misorientations During Coarsening in 2D Materials

When microstructure of polycrystalline materials undergoes coarsening driven by the elimination of energetically unfavorable crystals, a sequence of network transformations, including continuous expansion and instantaneous topological transitions, takes place. This talk will be focused on recent advances related to the mathematical modeling of this process. Two types of approaches will be discussed, one aimed at simulating the evolution of individual crystals in a 2-dimensional system via a vertex model focused on triple junction dynamics, and one providing a kinetic Boltzmann-type description for the evolution of probability density functions. The predicted MDF evolution based on the new kinetic mesoscale model will be discussed and contrasted with those obtained by large-scale phase field, MC and vertex simulations for several classes of interfacial energies.

Maria Emelianenko
George Mason University
memelian@gmu.edu

MS53

Parallel Octree-Based Discretizations for Diffusion Dominated Free Boundary Problems

The island dynamics model is a successful approach for simulating epitaxial growth. This model relies on the discretization of partial differential equations on Cartesian grids as well as the use of the level-set method. One of the main challenges when considering a level-set approach is to impose boundary conditions in a capturing framework, since the boundaries are not explicitly described. In addition, given the multiscale nature of epitaxial growth, where fine developing features need to be resolved, there is a need to consider efficient adaptive Cartesian discretizations and parallel strategies. In this talk, I will present recent advances in the numerical treatment of free boundary problems and parallel strategies.

Frederic G. Gibou
UC Santa Barbara
fgibou@engineering.ucsb.edu

MS53

Wetting and Dewetting Dynamics of Thin Solid Films

In this talk, we will discuss the dewetting dynamics of a thin solid film on a solid substrate when mass transport is controlled by surface diffusion. We show that the interaction with the substrate can lead to novel scenarios, such as a strong acceleration of the mass shedding process. Our findings are discussed within the light of recent experimental observations.

Oliver Pierre-Louis
Université Claude Bernard Lyon 1
olivier.pierre-louis@univ-lyon1.fr

MS54

An Upscaling Procedure for Passing from an Atomistic to a Continuum Model of Multi-Walled Carbon Nanotubes

A multi-walled carbon nanotube consists of several concentric tubes formed by graphene sheets—one-atom thick layers of carbon atoms arranged in a hexagonal lattice. A typical cross-section of a multi-walled tube can be modeled as several closed, nested, one-dimensional chains of atoms. In this talk, we present a rigorous atomistic-to-continuum procedure that upscales the energy of this discrete system of atoms to a continuum energy defined over curves in the plane. This continuum energy retains important atomistic information about lattice registry between the nested chains of atoms. In particular, the continuum model explains polygonization of cross-sections of large multi-walled nanotubes as a competition between the bending component of the energy and the component due to weak van der Waals interactions between adjacent walls.

Malena I. Espanol
Department of Mathematics
University of Akron
mespanol@uakron.edu

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

J. Patrick Wilber
Department of Mathematics
University of Akron
jw50@uakron.edu

MS54

Crystallization for a Brenner-Like Potential

The Brenner potential is used for carbon-carbon interactions in molecules such as graphene, carbon nanotubes, and diamond. We consider a Stillinger-Weber potential that is Brenner-like in two respects: (1) 180-degree bond angles are preferred, and (2) interactions are short range. We show that in two dimensions, the thermodynamic limit of the ground state energy per particle equals that of a honeycomb lattice. We also prove that, under periodic boundary conditions, the minimizers are honeycomb lattices.

Brittan A. Farmer

Department of Mathematics
University of Michigan
farbritt@umich.edu

Selim Esedoglu
University of Michigan
esedoglu@umich.edu

Peter Smereka
Department of Mathematics
University of Michigan
psmereka@umich.edu

MS54

A Framework to Compute Elastic Deformation Fields from Atomistics: the Key to Automated Identification of Dislocations, Grain Boundaries, and Stacking Faults

We describe a framework based on the Delaunay tessellation to compute the elastic deformation gradient field in 3d crystals containing defects from a set of input atomic coordinates. The method is being used in the analysis of molecular dynamics simulations of crystalline materials. Once the elastic mapping of the crystal to a perfect reference state has been established, key features such as dislocations, grain boundaries, and stacking faults can be identified in a rigorous and fully automated manner.

Alexander Stukowski
Technische Universität Darmstadt
stukowski@mm.tu-darmstadt.de

MS55

Spin Orbit Torques and Chiral Spin Textures in Ultrathin Magnetic Films

Spin orbit coupling at interfaces in ultrathin magnetic films can give rise to chiral magnetic textures such as homochiral domain walls and magnetic skyrmions, as well as current-induced torques that can efficiently manipulate them. This talk will describe interface-driven spin-orbit torques and Dzyaloshinskii-Moriya interactions (DMIs) in ultrathin ferromagnets adjacent to nonmagnetic heavy metals. We show that the DMI depends strongly on the heavy metal, differing by a factor of $\sim$20 between Pt and Ta, and describe the influence of strong DMI on domain wall dynamics and spin Hall effect switching. We then present high-resolution X-ray microscopy and scanning probe imaging of chiral magnetic skyrmions and their dynamics in multilayer films that allow the relevant energy terms to be engineered. Finally, we will describe how spin orbit torques can be enhanced through interface engineering and tuned by a gate voltage by directly controlling the interfacial oxygen coordination at a ferromagnet/oxide interface.

Geoffrey Beach
MIT
gbeach@mit.edu

MS55

Dynamical and Static Stabilization Mechanisms for Skyrmions

Topological defects such as domain walls and skyrmions have recently gained prominence as they owe their stability to their robustness against continuous deformations, similar to knots in a rope. Their stability renders them potentially useful for data storage applications similarly to other prominent topological defects such as domain walls in racetrack type memories. In view of the continuous demand of ever-increasing storage density it is important to study skyrmion-type defects on ever-decreasing length scales. Therefore it is necessary to understand the mechanisms which ensure the stability of skyrmions when their size becomes comparable to the crystal lattice and when thermal fluctuations are important. Here it will be discussed how dynamics can endow a skyrmion with stability even in the complete absence of Dzyaloshinskii-Moriya interactions which so far have been thought to be necessary to ensure the existence of skyrmions in ultrathin films.

Benjamin Braun
University of Kentucky
benjamin.braun@uky.edu

MS55

Current-Induced Dynamics of Chiral Skyrmions

Isolated chiral skyrmions occur in magnets without inversion symmetry as relative energy minimizers within a nontrivial homotopy class. We shall discuss their dynamic stability and effective dynamics governed by the Landau-Lifshitz-Gilbert equation including spin-transfer torque.

Christof Melcher
RWTH Aachen University
melcher@rwth-aachen.de

MS55

Ferromagnetic and Antiferromagnetic Skyrmions

Manipulating chiral spin textures, which can serve as bits of information, by electric current is one of the main challenges in the field of spintronics. Ferromagnetic skyrmions recently attracted a lot of attention because they are small in size and are better than domain walls at avoiding pinning while moved by electric current. Meanwhile, ferromagnetic skyrmions still have disadvantages such as the presence of stray fields and complicated transverse dynamics, making them harder to employ for spintronic applications. In this talk we also explore a related topological object: the antiferromagnetic (AFM) skyrmion. This topological texture has no stray fields and we show that its dynamics are faster compared to its ferromagnetic analogue. We obtain the dependence of AFM skyrmion radius on the strength of Dzyaloshinskii-Moriya interaction coming from relativistic spin-orbit effects and temperature. We find that the thermal properties, e.g. such as the AFM skyrmion radius and diffusion constant, are rather different from those for ferromagnetic skyrmions. More importantly, we show that due to unusual topology the AFM skyrmions do not have a velocity component transverse to the current and thus may be perfect candidates for spintronic applications.

Oleg Tretiakov
Tohoku University
Institute for Materials Research
olegt@imr.tohoku.ac.jp

MS56

On the Black-Hole Phenomenon at Corners of Metamaterials

In an appropriate frequency range, some metamaterials have electromagnetic constants with a small imaginary part and a negative real part. This leads to consider scattering

problems with sign-changing coefficients. An interesting phenomenon is the strongly oscillating behavior of the field that occurs at corners of such scatterer. In the 2D case, we show that a specific mathematical and numerical treatment is required, to capture this phenomenon and evaluate induced losses at the corners.

Anne Sophie Bonnet-Ben Dhia
ENSTA Paris Tech University
anne-sophie.bonnet-bendhia@ensta-paristech.fr

MS56

Spectral Properties of the Neumann-Poincaré Operator and Cloaking by Anomalous Localized Resonance for the Elasto-Static System

We first investigate spectral properties of the Neumann-Poincaré (NP) operator for the Lamé system of elastostatics. We show that the elasto-static NP operator can be symmetrized in the same way as that for Laplace operator. We then show that even if elasto-static NP operator is not compact even on smooth domains, its spectrum on tow dimensional smooth doamins consists of eigenvalues which accumulates to two numbers determined by Lamé constants. We then derive explicitly eigenvalues and eigenfunctions on disks and ellipses. We then investigate resonance occurring at eigenvalues and anomalous localized resonance at accumulation points of eigenvalues. We show on ellipses that cloaking by anomalous localized resonance takes place at accumulation points of eigenvalues.

Hyeonbae Kang
Department of Mathematics, Inha University
hbkang@inha.ac.kr

Kazunori Ando
Ehime Universtiy
ando@inha.ac.kr

Yongkwan Ji, Kyoungsun Kim
Inha University
22151063@inha.edu, kskim@inha.ac.kr

Sanghyeon Yu
ETH
sanghyeon.yu@sam.math.ethz.edu

MS56

Plasmonic Coupling Between Two Nanoparticles

We study the interaction between two closely located metallic nano-particles in two dimensions. We study the dependance of the plasmonic resonances with respect to the inter-particle distance. We show that the near-field stays bounded when the inter-particle distance goes to zero.

Pierre Millien
Ecole Polytechnique Federale de Lausanne
pierre.millien@epfl.ch

MS57

Formulations Treating Stochastic Effects in Thin Film Growth and Relaxation Including Contributions by Peter Smereka

Contributions by Peter to theory and modeling in materials science have been diverse and influential on topics including epitaxial thin film growth, film texture, coarsening theory, and grain growth. Often these recognized the importance of atomistic-level noise developing appropriate modeling formalisms. We describe some examples in thin film growth and relaxation, where stochastic effects are important for submonolayer island nucleation and growth shapes, for multilayer mound formation, and for post-deposition island coarsening.

James Evans
Ames LaboratoryUSDOE
Dep of Physics & Astro and Dep of Math, Iowa State Univ
evans@ameslab.gov

MS57

A Levelset Method for Modeling the Formation and Self-Organization of Quantum Dots During Epitaxial Growth

Strain is often the driving force behind the formation and self-organization of quantum dots and other nanoscale structures during epitaxial growth. It is therefore of paramount importance to understand and to be able to model epitaxial growth of strained system. In this talk we will discuss a model for epitaxial growth that employs an island dynamics model with the level-set technique in combination with a fully self-consistent elastic model that has been developed and implemented by Peter Smereka. In the island dynamics model islands are treated as continuous in the x-y-plane, while individual atomic layers are resolved in the z-direction. Adatoms are treated as a mean field quantity by solving a diffusion equation. The relevant (microscopic) input parameters for our model can be obtained from density-functional theory calculations. We will present results for several growth phenomena: In the submonolayer growth regime, islands become smaller and more regular upon increasing strain, and the island size distribution narrows and sharpens. We will discuss how a spatially varying potential energy surface for adatom diffusion can be exploited for pattern formation. Such spatial variations are for example a result of defects or other features that are buried under the substrate. Another example is the growth of stacked quantum dots, where islands self-align on top of previously grown islands.

Christian Ratsch
UCLA
Department of Mathematics
cratsch@math.ucla.edu

MS57

Kinetic Monte Carlo—A Look Back and a Glance Forward

In this talk I will review the work Peter and I did together on Kinetic Monte Carlo (KMC). Most of this focused on applications to hetero-epitaxial growth, where the challenge is to introduce elastic effects into the model. This requires either an off-lattice or lattice-plus-displacement-field approach, either of which involves rate computations that are orders of magnitude more costly than required for more conventional lattice-based KMC simulations. I will focus on two techniques that were especially important in overcoming this bottleneck: a rejection scheme using rate estimates similar to the bond-counting models typically used in lattice-based KMC and a local approximation that proved to be more accurate than one would naively expect. Finally, I will discuss the prospects for expanding

upon these methods in the future.

Tim Schulze
University of Tennessee
Department of Mathematics
schulze@math.utk.edu

MS57

Phase Field Models Capturing Surface Diffusion

Phase field models are robust numerical tools to solve free boundary problems corresponding to the motion of interfaces. Also for interface motion via surface diffusion various phase field models have been suggested. A promient example is the Cahn-Hilliard equation with a degenerate mobility function. We discuss versions which do and versions which don't converge asymptotically to the sharp interface limit. We further extend the approach to consider strong anisotropic surface diffusion leading to faceted structures and show applications in the context of heteroepitaxial growth and solid state dewetting.

Axel Voigt
TU Dresden
axel.voigt@tu-dresden.de

MS58

Multi-scale Atomistic Simulations Scheme for Grain Boundaries

To simulate the interaction of solutes with general grain boundaries we present an improved method for embedding a quantum mechanical system inside a larger classically treated domain. This allows the resolution of interesting electronic effects while capturing the long range behavior. The approach is illustrated for calculating binding energies of Pb to grain boundaries in Al, i.e. a Sigma 5 boundary to benchmark against fully-periodic density functional theory and a general tilt boundary.

Liam Huber, Blazej Grabowski, Joerg Neugebauer
Max-Planck-Institute for Iron Research
liam.huber@gmail.com, bgrabowski@mpie.de,
neugebauer@mpie.de

Joerg Rottler, Matthias Militzer
University of British Columbia
j.rottler@phas.ubc.ca, matthias.militzer@ubc.ca

MS58

Review of Abnormal Grain Growth, New and Old Mechanisms

The wide variety of circumstances and mechanisms that lead to abnormal grain growth are reviewed such as subgrain networks and heterogeneous stored energy. Two in particular are highlighted. For grain sizes below the Smith-Zener limit of particle pinning, grains can grow abnormally. Then in systems that exhibit complexion transitions, grains that acquire sufficient perimeter of high mobility boundaries can become abnormal. Current evidence points to propagation of complexions through triple lines.

Anthony Rollett
Carnegie Mellon University
Materials Science and Engineering
rollett@andrew.cmu.edu

MS58

Twin Boundary Junction Effects in Grain Growth

Twinning readily occurs during grain growth in face centered cubic materials and twin junction formation is a natural consequence. We examine the role grain boundary migration plays in twin junction formation and the impact of twin junctions on subsequent grain growth via molecular dynamics simulation of nanocrystalline Ni. Of these junctions, penta-twins are particular interesting; we examine their disclination character and their impact on boundary migration.

David J. Srolovitz, Spencer Thomas
University of Pennsylvania
srol@seas.upenn.edu, slthomas61@gmail.com

MS59

A Mathematical Analysis of the GW Method for Computing Electronic Excited Energies

The aim of this presentation is to provide a mathematical framework for the GW approximation used to compute excited states in molecules or band-gaps in solids. I will first make precise the properties of Green's functions, which are one-body operators that naturally appear in many-body perturbation theory. I will then give a rigorous mathematical formulation of various GW schemes, such as the GW_0 equations for molecules, and study their well-posedness – for instance by showing the existence of a unique solution in a perturbative regime.

Gabriel Stoltz
CERMICS
Ecole des Ponts ParisTech
stoltz@cermics.enpc.fr

MS59

Ab Initio Parametrization of Bond-polarizability Model for Raman Spectroscopy of a-Si:H

Classical molecular dynamics with inter-atomic potentials can be quite successful at predicting the vibrations of materials, and is especially useful for handling large structural models (e.g. tens of thousands of atoms) that are intractable by quantum methods. However, to predict Raman spectra, electrons must be re-introduced to the problem via a model for the polarizability and its variation with atomic positions. The established approach for bulk semiconductors is to construct a bond-polarizability model, attributing the polarizability to cylindrically symmetrical inter-atomic bonds. Using an assumed form for the polarizability as a function of bond length, the parameters are fit to experimental data. Then, a Raman intensity can be computed for the vibrational eigenvectors from classical potentials. However, in the case of amorphous silicon, use of the existing models with vibrational eigenvectors from DFT has shown significant discrepancies from experiment [R. M. Ribeiro et al., phys. stat. sol. (c) 7, 1432 (2010)]. By contrast we find that the Raman spectrum calculated by density-functional perturbation theory for a set of 64-atom a- Si:H structures agrees well with the measured spectrum. These results suggest that the models have compensated errors in the classical vibrational frequencies with errors in the Raman tensors. To generate a more accurate and transferable bond polarizability model, we fit a general

bond-polarizability model to the ab initio atomic Raman tensors in our data set to obtain parameters and functional forms that can describe the Raman intensities of vibrations in large structural models. This new Raman model can be used to study problems such as medium- and long-range order in a- Si:H, nanocrystalline Si, amorphous/crystalline interfaces, or a-Si:H nanowires at sizes that would be inaccessible for ab initio vibrational calculations, and offers the potential to apply the same methodology to other material systems.

David A. Strubbe, Jeffrey C. Grossman
Department of Materials Science and Engineering
Massachusetts Institute of Technology
dstrubbe@mit.edu, jcg@mit.edu

MS59

A New Algorithm for Real-time Time Dependent Density Funcitonal Theory Calculations

In this talk, I will present our new algorithm for a real-time time dependent density funcitonal theory (rt-TDDFT) simulation. This algorithm can be used to simulate a 100 atom system for up to one ps using plane wave basis set. I will compare this method with the conventional propagation based method. I will also discuss the numerical convergence issue of this method, and our efforts to introduce a decay mechanism in the Ehrenfest dynamics. The current method has been used to study ion-substrate collision, hot carrier cooling in quantum dot, and plasmon excitation in metal nanoclusters.

Lin-Wang Wang
Lawrence Berkeley National Lab
lwwang@lbl.gov

MS60

Geometry and Topology of Turbulence in Active Nematics

The problem of low Reynolds number turbulence in active nematic fluids is theoretically addressed. Using numerical simulations, I demonstrate that an incompressible turbulent flow, in two-dimensional active nematics, consists of an ensemble of vortices whose areas are exponentially distributed within a range of scales. Building on this evidence, I construct a mean-field theory of active turbulence by which several measurable quantities, including the spectral densities and the correlation functions, can be analytically calculated. Because of the profound connection between the flow geometry and the topological properties of the nematic director, the theory sheds light on the mechanisms leading to the proliferation of topological defects in active nematics and provides a number of testable predictions. A hypothesis, inspired by Onsagers statistical hydrodynamics, is finally introduced to account for the equilibrium probability distribution of the vortex sizes.

Luca Giomi
Universiteit Leiden
giomi@lorentz.leidenuniv.nl

MS60

Nonlinear Spatiotemporal Dynamics of Active Fluids and Applications to Cell Biomechanics

Abstract not available at time of publication.

Rajesh Ramaswamy
MPI Physics of Complex Systems
rrajesh@pks.mpg.de

MS60

A Hybrid Particle-Mesh Method for Incompressible Active Polar Viscous Gels

Abstract not available at time of publication.

Ivo F. Sbalzarini
TU Dresden, Computer Science
& MPI Molecular Cell Biology & Genetics
ivos@mpi-cbg.de

MS61

Increasing the Timestep in Molecular Dynamics Simulation

Materials models formulated with all-atom potentials are typically simulated using molecular dynamics. I will discuss ongoing efforts to improve the efficiency of timestepping methods for molecular dynamics simulation. The allowable simulation timestep depends on the structure of the molecular system under study. I will describe stochastic, constraint-preserving schemes designed to increase the allowable stepsize. I will also discuss trade-offs between methods that provide dynamical fidelity (the calculation of reaction or diffusion rates) and schemes meant to provide good approximation of long term averages.

Ben Leimkuhler
University of Edinburgh
School of Mathematics
b.leimkuhler@ed.ac.uk

MS61

On the Numerical Treatment of Dissipative Particle Dynamics and Related Systems: An Adaptive Formulation

We review and compare numerical methods for particle-based models, in particular, dissipative particle dynamics (DPD) as well as a newly proposed stochastic pairwise adaptive Langevin (PAdL) method that fully captures the dynamics of DPD. Splitting methods are developed and studied in terms of their thermodynamic accuracy, two-point correlation functions, and convergence. We report significant advantages in computational efficiency for the PAdL method compared to popular alternative schemes in both equilibrium and nonequilibrium simulations.

Xiaocheng Shang, Benedict Leimkuhler
University of Edinburgh
x.shang@ed.ac.uk, b.leimkuhler@ed.ac.uk

MS61

Error Analysis of Modified Langevin Dynamics

We consider Langevin dynamics associated with a modified kinetic energy vanishing for small momenta. This allows us to freeze slow particles, and hence avoid the recomputation of inter-particle forces, which leads to computational gains. On the other hand, the statistical error may increase since there are a priori more correlations in time. The aim of this work is first to prove the ergodicity of the modified Langevin dynamics (which fails to be hypoelliptic), and next to analyze how the asymptotic variance on ergodic averages depends on the parameters of the

modified kinetic energy. Numerical results illustrate the approach, both for low-dimensional systems where we resort to a Galerkin approximation of the generator, and for more realistic systems using Monte Carlo simulations.

Zofia Trstanova
Inria
zofia.trstanova@inria.fr

Gabriel Stoltz
ENPC, Paris
gabriel.stoltz@enpc.fr

Stephane Redon
Inria
France
stephane.redon@inria.fr

MS61

Coarse-Graining Strategies for Polymer Systems

Existing coarse-graining methods based on uncontrolled closures, such as the "Iterative Boltzmann Inversion", intend to match structural properties, but exhibit significant discrepancies in thermodynamic quantities. Alternatively, one can obtain an "ideal" coarse-grained model by integrating all atomistic degrees of freedom for a given coarse-grained configuration. This would give an exact but complicated expression for the coarse-grained potential. However, in some cases, this is computationally tractable and can provide good control on both structural and thermodynamical properties.

Dimitrios Tsagkarogiannis
Department of Applied Mathematics University of Crete
D.Tsagkarogiannis@sussex.ac.uk

Anastasios Tsourtis, Vagelis Harmandaris
University of Crete
tsourtis@uoc.gr, harman@uoc.gr

MS62

Infinite-Order Laminates in a Crystal Plasticity Model with Two Slip Systems

The macroscopic material response of certain crystalline solids appears to be largely influenced by the spontaneous formation of microstructure as the material responds locally to internal stresses. We'll discuss a variational model for an elastically rigid crystalline structure in which the crystalline lattice can slip in two orthogonal directions. By exploring the generalized convex envelopes of the local energy, we make some qualitative observations related to spontaneous microstructure formation.

Nathan Albin
Kansas State University
albin@math.ksu.edu

MS62

Multiscale Structure of Optimally Designed Composites with Nonlocal Constitutive Relations

Optimization of the structure of materials with nonlocal constitutive relations is formulated as a min-max optimization problem for uncertain or stochastic loadings. Geometric parameters of an optimally designed composite are related to the parameters of the nonlocal constitutive equation through the spectral measure in the Stieltjes integral representation of the effective properties. This allows us to find the optimal structural parameters using solution of the min-max problem.

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

MS62

The Rheology of Non-Dilute Dispersions of Highly Deformable Viscoelastic Particles in Newtonian Fluids

We present a model for the rheological behavior of non-dilute suspensions of initially spherical, viscoelastic particles in viscous fluids under uniform, Stokes flow conditions. The particles are assumed to be neutrally buoyant, Kelvin-Voigt solids undergoing time-dependent, finite deformations, and exhibiting generalized neo-Hookean behavior in their purely elastic limit. We investigate the effects of the shape dynamics and constitutive properties of the viscoelastic particles on the macroscopic rheological behavior of the suspensions.

Pedro Ponte Castaneda
University of Pennsylvania
ponte@seas.upenn.edu

MS63

Active Mechanics of Spindle Positioning

The position of the spindle determines the position of the cleavage plane during cell division, and is thus of critical importance in development. We are investigating how different forces coordinated to move the spindle, and if these forces are generated from interactions with the cytoplasm, the cortex, or a combination of both. We are studying these issues using quantitative experiments: including a novel laser ablation systems to quantitatively perturb spindle movements and fluorescent nanodiamonds to track fluid flows as the spindle moves. We are attempting to interpret our results through comparison with simulations and theory.

Dan Needleman
School of Engineering and Applied Sciences
Harvard University
dan.needleman@gmail.com

MS63

Modeling Dynamics of and Within the Mitotic Spindle

Abstract not available

Michael J. Shelley
New York University
Courant Inst of Math Sciences
shelley@cims.nyu.edu

MS63

Confined Spherical Polymer Micelle in a Tube Tunnel

Phase behavior of the blends composed of diblock copolymer (AB) and homopolymer (A) micelles confined in a

tube tunnel was studied using the self-consistent field theory. AB diblock copolymer and A homopolymer blend can form micelles of different shapes (lamellar, cylindrical, and spherical) because they have different critical micelle concentration (CMC). According to the CMC, we can find a stable spherical micelle morphology with a set of molecular parameters. When the spherical polymer micelle was confined in a channel, the shape of the micelles may differ from that of the bulk micelles. We study the shape variation of a spherical micelle under confinement with different A-homopolymer length. The results reveal depletion effect and capillary condensation. And these results are consisted with the physical experiment.

Hui Zhang
Beijing Normal University
hzhang@bnu.edu.cn

MS64

Formation of Moire Patterns in Ultra Thin Heteroepitaxial Films

When an ultrathin film is deposited on a surface, the interaction of the film and substrate can lead to interesting patterns or superstructures within the film. In this talk I would to discuss the influence of misfit strain, adhesion strength and lattice symmetry on the complex Moire patterns that form when films of triangular symmetry are adsorbed on compact triangular or honeycomb substrates.

Ken Elder
Dept Physics
Oakland U.
elder@oakland.edu

MS64

From Atomistic Dynamics to Mesoscale Descriptions of Crystal Growth

At the microscopic scale, epitaxial growth is usually described by the atomistic dynamics of diffusion-like processes in the context of solid-on-solid models and the kinetic Monte Carlo method. At the mesoscale, the morphological evolution of crystal surfaces is described via the motion of nanoscale defects, steps, in terms of suitable free-boundary problems. In recent years, there have been research efforts to connect the two descriptions. In this talk, I plan to discuss recent progress and challenges in this direction.

Dionisios Margetis
University of Maryland, College Park
dio@math.umd.edu

MS65

Magnetism Pathways in Transition Metal Substituted Graphene: A DFT study

Abstract not available

Costel Constantin
James Madison University
constacx@jmu.edu

MS65

A Bending Theory for Nematic Elastomers

Nematic liquid crystal elastomers couple the elasticity of a polymer network with the anisotropy of liquid crystal molecules. The result is a solid displaying unique phenomena such as soft elasticity, spontaneous distortion and microstructure. We derive a bending type theory for thin sheets of this material via Γ-convergence assuming entropic and Frank elasticity are comparable in this regime. Many interesting features emerge from this theory, including spontaneous curvature and a design principal for active nematic glass sheets.

Paul Plucinsky
California Institute of Technology
pplucins@caltech.edu

Kaushik Bhattacharya
Howell N. Tyson Sr. Professor of Mechanics
California Institute of Technology
bhatta@caltech.edu

MS65

Coarse-Grained Modeling and Simulations of a Carbon Nanotube Forest Interacting with a Rigid Substrate

Abstract not available

J. Patrick Wilber
Department of Mathematics
University of Akron
jw50@uakron.edu

MS66

Structure, Stability and Existence of 360 Degree Walls

In this talk we study a variational micromagnetic model in the thin film and relatively soft regime, where the energy features exchange, anisotropy and stray-field energy terms. The aim is to present some results about the existence and structure of one-dimensional 360 degree Nel walls, such that the transition direction of the walls makes an angle α with respect to the easy axis. Depending on this angle we show, besides existence or non existence, some properties about the the structure of such domain walls.

Antonio Capella Kort
Universidad Nacional Autónoma de México
capella@matem.unam.mx

Hans Knuepfer
University of Heidelberg
knuepfer@uni-heidelberg.de

Cyrill B. Muratov
New Jersey Institute of Technology
Department of Mathematical Sciences
muratov@njit.edu

MS66

Charged Boundary-Layer Domain Walls in Thin Ferromagnetic Films

Ultrathin ferromagnetic films are known to exhibit a rich variety of magnetization patterns in which the magnetization vector remains almost entirely in the film plane. In this talk, I will discuss a particular regime governed by a competition of the exchange, stray field and Zeeman energies. Using the techniques of Γ-convergence, we de-

scribe the limit behavior of the energy minimizers exhibiting charged boundary domain walls as the film thickness goes to zero while the film's lateral extent goes to infinity with a suitable rate.

Ross Lund
NJIT
ross.lund@gmail.com

Cyrill B. Muratov
New Jersey Institute of Technology
Department of Mathematical Sciences
muratov@njit.edu

Valeriy Slastikov
University of Bristol
Bristol, UK
Valeriy.Slastikov@bristol.ac.uk

MS66

Domain Wall Dynamics in Magnetic Nanostructures

We discuss some recent analytic results concerning domain wall dynamics in one-dimensional magnetic nanowires and nanotubes, including existence of travelling waves under applied fields and currents, bifurcations to oscillatory and KPP-type behaviour, and effects of Dzyaloshinskii-Moriya interactions.

Arseni Goussev
Northumbria University
arseni.goussev@northumbria.ac.uk

Ross Lund
NJIT
ross.lund@gmail.com

Jonathan Robbins
University of Bristol
j.robbins@bristol.ac.uk

Valeriy Slastikov
University of Bristol
Bristol, UK
Valeriy.Slastikov@bristol.ac.uk

Oleg Tretiakov
Tohoku University
Institute for Materials Research
olegt@imr.tohoku.ac.jp

S Vasylkevych
University of Bristol
s.vasylkevych@bristol.ac.uk

MS66

Dynamics in Strongly Spin-Torque-Driven Magnetic Thin Film Nano-Structures

I review the basic constitutive relationships governing the dynamics of a nanomagnet under the influence of spin-torque drive at a magnitude well above its instability threshold. Starting from the Landau-Lifshitz-Gilbert-Slonczewski Equation and a macrospin assumption, I will build a simple and intuitive physical picture of the process, with the presence of finite temperature. I will then discuss some real-world behaviors beyond what such a simple model can capture. Chief among them the finite exchange-interaction related length-scale issues, and the experimental observations related to such. These will be discussed within the context of optimizing a spin-torque-based nanoamagnet switch for the application of CMOS-integrated random access memory technology. I acknowledge project funding and fruitful collaboration with our joint-technology-development partners including Samsung Electronics, Micron Technology, and TDK-Headway.

Jonathan Sun
IBM
jonsun@us.ibm.com

MS67

Weyl Modes and Periodicity-Changing Mechanisms in Mechanaical Metamaterials

Recent work on topological invariants of phonon bands in mechanical systems has led to the design of localized zero-energy modes at boundaries and dislocations in special ball-spring lattices, beam structures, and even origami. We present the results of theory and simulations on periodic mass spring lattices admitting topologically-protected zero-energy bulk modes, called Weyl modes, after analogous modes in electronic systems. We demonstrate how these lead to mechanisms that alter the periodicity of the unit cell.

Bryan G. Chen
University of Massachussetts
bryanchen@umass.edu

David Zeb Rocklin
University of Michigan
drocklin@umich.edu

Martin Falk
MIT
falkma@sas.upenn.edu

Vincenzo Vitelli
Associate Professor,Soft Condensed Matter Theory Group
Instituut-Lorentz, Universiteit Leiden
vitelli@lorentz.leidenuniv.nl

Tom Lubensky
University of Pennsylvania
tom@physics.upenn.edu

MS67

High Frequency Homogenization for Traveling Waves

Here we employ the high frequency homogenization methods of Craster, Kaplunov and Pichugin to travelling wave packets in periodic media. As expected we find that the wavepackets satisfy a first-order partial differential equation characteristic of travelling waves at the group velocity. The approach works for the Helmholtz equation, Schrodinger equation, Maxwell's equations, and the elastodynamic equation. The results are in accord with work of Allaire, Palombaro, Rauch and Piatnitski.

Davit Harutyunyan
University of Utah
davith@math.utah.edu

Graeme W. Milton
University of Utah
Department of Mathematics
milton@math.utah.edu

Richard Craster
Department of Mathematics
Imperial College London
r.craster@imperial.ac.uk

MS67

On Scattering Resonances of Subwavelength Metallic Gratings

The talk is aimed at understanding the amplification and confinement of electromagnetic fields in open subwavelength metallic gratings. We present a theoretical study of the electromagnetic diffraction by a perfect or a real metallic planar interface which contains subwavelength rectangular cavities. We derive a rigorous asymptotic expansion of the scattering resonances when the width of the cavities tend to zero.

Faouzi Triki
Universite Joseph Fourier, Grenoble
Laboratoire Jean Kuntzmann
faouzi.triki@imag.fr

Eric Bonnetier
Université Joseph Fourier, Grenoble
Laboratoire Jean Kuntzmann
eric.bonnetier@imag.fr

Abdelfettah Gtet
Université Joseph Fourier, Grenoble Laboratoire Jean Kuntzma
abdelfettah.gtet@imag.fr

MS67

Electromagnetic Waves in 2D Honeycomb Structures

We first discuss results on the novel dispersion properties, such as Dirac points in the band structure, of Maxwells equations in media with honeycomb symmetry. We then discuss "edge states", electromagnetic modes which propagate parallel to a line defect in the bulk structure and are localized transverse to it. We focus, in particular, on edge states which are topologically protected. These results extend earlier results on the Schrödinger equation of CL Fefferman, JP Lee-Thorp and MI Weinstein.

James P. Lee-Thorp
Columbia University
jpl2154@columbia.edu

Michael I. Weinstein
Columbia University
Dept of Applied Physics & Applied Math
miw2103@columbia.edu

Yi Zhu
Zhou-Pei-Yuan Center for Applied Mathematics
Tsinghua University, China
yizhu@mail.tsinghua.edu.cn

MS68

Modeling Elastic Energy of Alloys: Potential Pitfalls of Continuum Treatments

Continuum theories are widely used to model the elastic energy due to compositional/configurational strain in alloys. The most common approach is to posit an effective misfit that depends on the local composition of the crystal. This composition is in turn assumed to vary on a macroscopic scale. This talk will discuss some crucial issues in modeling the elastic energy of alloys using this approach. In particular it will be shown through an exact solution of the Ball and Spring (Keating) model that such a continuum theory fails to capture the elastic energy of alloys. This is due to the lack of account of microscopic re-arrangements of atoms. The results of the ball and spring model show that finely mixed alloys have a higher elastic energy, the exact opposite of the prediction by continuum theories. The results are further substantiated using electronic density functional theory calculations.

Arvind Baskaran
University of California, Irvine
baskaran@math.uci.edu

Christian Ratsch
UCLA
Department of Mathematics
cratsch@math.ucla.edu

Peter Smereka
Department of Mathematics
University of Michigan
psmereka@umich.edu

MS68

Examining Two-dimensional Ordering from Isotropic Interactions

In this talk I would like to discuss the generic mechanisms driving the formation of two dimensional crystal structures. More specifically I will focus on how the interaction of three length scales can give rise to all five two-dimensional bravais lattices and many more complex structures including honeycomb, kagome, dimer and even systems with chiral symmetry.

Ken Elder
Dept Physics
Oakland U.
elder@oakland.edu

Simiso Mkhonta
Dept. of Physics
University of Swaziland
simiso.mkhonta@wayne.edu

Zhi-Feng Huang
Dept Physics
Wayne State University
huang@physics.wayne.edu

MS68

Large Scale Simulations for a Simple Recrystalliza-

tion Model via Diffusion Generated Motion

We simulate a classical model of recrystallization in unprecedented detail and in physically relevant parameter regimes not attainable with many previous numerical techniques.

Selim Esedoglu
University of Michigan
esedoglu@umich.edu

Matt Elsey
Courant Institute
New York University
melsey@cims.nyu.edu

Peter Smereka
Department of Mathematics
University of Michigan
psmereka@umich.edu

MS68

Sensitivity and Parametrization for Multiscale KMC Simulations

We present an overview of methods based on information-theoretic tools for estimating parametric sensitivities in multiscale models simulated by kinetic Monte Carlo. We discuss stochastic averaging in systems with multiple time scales and its application to obtaining bounds on sensitivity indices. Furthermore, we show how the path-space relative entropy allows us to formulate a variational inference problem for obtaining parametrization of transition rates in coarse-grained models in systems with non-equilibrium steady states.

Petr Plechac
University of Delaware
Department of Mathematical Sciences
plechac@math.udel.edu

MS69

Study the Formation of Microstructure for Highly Reversible Martensitic Materials

Martensitic materials are exploited for emerging applications in medical devices, microelectronics and energy conversion devices. However the functionalities of these martensitic materials usually degrades significantly after only few transformation cycles. The origin of such degradation comes from the formation of microstructure consisting stressed-transition layers due to lattice mismatch at heterophase boundaries. It has been proven that when the lattice parameters satisfy the conditions of compatibility, both hysteresis and reversibility can be optimized, thus long life-time is achieved for these applications. New alloys discovered by satisfying these conditions exhibit exceptional reversibility and low hysteresis, i.e. zero functional migration up to millions cycles. In sharp contrast to ordinary martensitic materials, a variety of hierarchical microstructures arises in these highly reversible materials: curved and zig-zag interfaces. In addition, the material loses the usual reproducibility and acoustic emission traces from cycle to cycle. Here, we would like to present the formulation of the geometric conditions of compatibility and their roles in discovering highly reversible materials. We have developed an approach for observation of the formation of interface by *in situ* micro-Laue scan. Combined with the theoretical calculation, the mysteries of unusual hierarchies in the highly reversible material can be understood.

Xian Chen
The Hong Kong University of Science and Technology
xianchen@ust.hk

MS69

Atomistic-to-Continuum Coupling for Multilattices Through Blending

The blended force-based quasicontinuum method is an atomistic-to-continuum method used to model defects by modelling regions near the defect with an atomistic model and modeling the elastic far-fields with a continuum model. Forces on degrees of freedom in the atomistic and continuum regions are defined and smoothly blended together. We introduce this method for multilattices and describe decay rates for the fully atomistic model needed to construct an optimally graded mesh for the continuum model.

Derek Olson
School of Mathematics
University of Minnesota
olso4056@umn.edu

Xingjie Li
University of North Carolina at Charlotte
xli47@uncc.edu

Christoph Ortner
University of Warwick
c.ortner@warwick.ac.uk

Mitchell Luskin
School of Mathematics
University of Minnesota
luskin@math.umn.edu

MS69

A Kinetic Monte Carlo Model for Grain Boundary Motion Driven by Curvature

The evolution of grain boundary networks is typically done using continuum models or Potts models, both of which are aimed at length scales containing large numbers of individual grains. At the atomistic scale, molecular dynamics can be used to study the interaction of a few grains, but at great computational cost. Further, one often needs to assume artificially high temperatures to use this approach. In this talk, I will discuss a lattice-based kinetic Monte Carlo model aimed at studying atomistic scale grain boundary evolution. I will present some simulations of two-grain systems that are able to capture both the motion by curvature behavior that continuum models are based upon and the break-down in this behavior that is revealed in molecular dynamics simulations. Mechanisms for the existence of this growth law and for its failure at small length scales will be discussed.

Tim Schulze
University of Tennessee
Department of Mathematics
schulze@math.utk.edu

Kyle Golenbiewski
University of Tennessee

kyle@math.utk.edu

MS69

A Peierls-Nabarro Model of Semicoherent Interfaces

Interfaces between different materials can be very complex. When the two materials have structures and lattice parameters that nearly match on particular planes, the interfaces can be described by a set of dislocations that may form complex patterns. We employ a generalized Peierls-Nabarro model that predicts the structure and energetics of such interfaces, including these complex line defect structures. In particular, we show how misfit transform dislocation node structures.

David J. Srolovitz, Shuyang Dai
University of Pennsylvania
srol@seas.upenn.edu, shuyangd@seas.upenn.edu

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

MS70

Directed Self-Organization with Long-Range Forces: A Dynamical Approach

A strained film coherently deposited on a substrate undergoes a morphological instability driven by surface diffusion that eventually evolves into self-organized quantum dots. We study the evolution of this instability on a patterned substrate. If coarsening usually leads to disordered objects, the growth on a patterned substrate leads in some conditions to uniform arrays of dots which locate in different configurations depending on the experimental conditions. We characterize the dynamics of such a directed self-organization.

Jean-Noel Aqua
Institut des NanoSciences de Paris
aqua@insp.jussieu.fr

MS70

Thin Film De-Wetting in the Presence of Long-Range and Oscillatory Interactions

Long range de-wetting forces acting across thin films, e.g., van der Waals interactions, may drive the formation of large clusters observed in thin films. These interactions introduce a distinct long lasting early-time scaling behavior characterized by a slow growth of the cluster height/lateral size aspect ratio (i.e., a time-dependent Young angle), and by effective coarsening exponents that depend on cluster size. We analytically calculate these effective exponents characterizing the cluster growth in the early-time regime.

Leonardo Golubovic
West Virginia University
leonardo.golubovic@mail.wvu.edu

MS70

Phase Transition Fronts in Systems with Subdiffusion

Subdiffusive transport has been detected in numerous physical and biological systems, specifically in gels. In the present talk, we consider two problems where the role of subdiffusion is significant. The first example is the growth of a solid nucleus in a supersaturated gel. The second example is the dissolution of a solid particle (glass/gel transition) when the solvent is subjected to subdiffusion. We obtain exact self-similar solutions describing propagation of the phase-transition fronts and discuss their stability.

Alexander Nepomnyashchy
Technion
Israel Institute of Technology
nepom@math.technion.ac.il

Vladimir A. Volpert
Northwestern University
v-volpert@northwestern.edu

MS70

G-Equivariant Theory of Coarsening Beyond the Dynamic Scaling Hypothesis

We propose that the dynamical symmetries of coarsening dynamical systems necessarily covariantly act on the statistics of the resultant coarsening texture. We exhibit this thesis for a model chiral dynamics (Watson SJ. 2015) which coarsens two enantiomerically related phases while preserving the *enantiomeric excess*. Here the dynamical symmetry group is found to contain not only a parabolic spatio-temporal scaling, but also a Lorentzian boost which acts non-trivially on the phase-fraction. We thereby theoretically predict the exact analytical dependence of the characteristic domain length on both time and the invariant phase fraction. Reference: Watson SJ. "Emergent parabolic scaling of nano-faceting crystal growth". Proc. R. Soc. A 471, 20140560 (2015).

Stephen J. Watson
University of Glasgow
Stephen.Watson@glasgow.ac.uk

MS71

Converting Strain Maps into Elasticity Maps for Materials with Small Contrast

Session Code: I This study focuses on the quantitative reconstruction of heterogeneous distributions of isotropic elastic moduli from full strain field data. A local reconstruction procedure is investigated here in the case of materials with small contrast. Within the framework of the integral formulation of the linear elasticity problem, first-order asymptotics are retained for the strain field solution and the effective elasticity tensor. Properties of the featured infinite-body Greens operator are investigated to characterize its local and non-local contributions to the volume integral equations considered. The former is then shown to coincide with the isotropic component of the Greens tensor. Based on this property, the combination of multiple strain field solutions corresponding to well-chosen applied macroscopic strains is shown to yield a set of local and uncoupled equations relating, respectively, bulk and shear moduli to the spherical and deviatoric components of the strain fields. Valid for any material configuration at first-order in the small contrast limit, such relations permit a pointwise conversion of strain maps into elasticity maps. Furthermore, for isotropic geometries it is also shown that a single strain field solution is actually needed to reconstruct either the bulk and the shear modulus distributions. A set of examples illustrates the use of these local equations

for parameters identification from full-field data.

Cedric Bellis
Ecole Polytechnique, France
bellis@lma.cnrs-mrs.fr

Pierre M. Suquet
CNRS
Laboratoire de Mecanique et d'Acoustique
suquet@lma.cnrs-mrs.fr

MS71

Increasing Stability for Inverse Problems

The problem of recovering conductivity from boundary measurements has been studied since the 1980s. It is well known that a logarithmic stability estimate holds and is optimal. However, the logarithmic stability makes it difficult to design reliable reconstruction algorithms in practice since small errors in the data of the inverse problem result in large error in numerical reconstruction of physical properties of the medium. It has been observed numerically that the stability improves if one increases the frequency in some cases. The main purpose of this talk is to discuss several results which rigorously demonstrate the increasing stability behavior in different settings.

Ru-Yu Lai
University of Minnesota
rylai@umn.edu

MS71

New Methods for Imaging

Here we establish a direct connection between the Dirichlet to Neumann map governing the response of bodies and the abstract theory of composite materials. As a result methods for bounding the effective tensors of composites can be applied to bounding the Dirichlet to Neumann map and these can be used in an inverse way to obtain information about the geometry inside the body. Specifically we show how bounds using the translation method for bounding the effective moduli can be used to bound the Dirichlet to Neumann map and how bounds on the transient response of composites (obtained with Ornella Mattei) can be extended to bodies, using analytic properties of the Dirichlet to Neumann map as a function of the component moduli: for electromagnetism these analytic properties were established with Maxence Cassier and Aaron Welters

Graeme W. Milton
University of Utah
Department of Mathematics
milton@math.utah.edu

MS72

Connecting Atomistic and Continuum Models of Nonlinear Elasticity

I will discuss how (classical) models of atomic interactions and continuum nonlinear elasticity are connected by the Cauchy-Born rule in a crystalline solid. In particular, I will present a result on the existence of solutions to the atomistic problem and their convergence to a solution of the continuum model as the interatomic distances tend to zero. This is done in a dynamical setting with long term existence and Dirichlet boundary conditions.

Julian Braun
University of Augsburg
Institut fuer Mathematik
julian.braun@math.uni-augsburg.de

MS72

Derivation of Self Interaction Energy for Dislocations

I will present the derivation, in terms of Gamma-convergence, of three-dimensional variational models for material defects and crystal plasticity. Depending on the energy scaling one can obtain a line tension energy associated to dislocations in 3D or a gradient theory for plasticity. The rigorous analysis shows that in some cases the effective models may reveal the presence of relaxation and formation of microstructure.

Sergio Conti
Institut fur Angewandte Mathematik
Universitat Bonn
sergio.conti@uni-bonn.de

Adriana Garroni
Universita' di Roma
garroni@mat.uniroma1.it

Stefan Mueller
University of Bonn
stefan.mueller@hcm.uni-bonn.de

Michael Ortiz
California Institute of Technology
ortiz@aero.caltech.edu

MS72

Convergence of Interaction-Driven Evolutions of Dislocations

It is well known that the plastic, or permanent, deformation of a metal is caused by the movement of curve-like defects in its crystal lattice. These defects are called dislocations. What is not yet clear is how to use this microscale information to make theoretical predictions at the continuum scale. Motivated by this, we considered systems of interacting dislocations and studied the convergence of the evolutions of the corresponding empirical measures in the limit of many dislocations. In the continuum limit we obtained evolution laws for the dislocation density. In this talk I will present these results and discuss their limitations and further extensions towards more realistic and complex systems. The results above have been obtained in collaboration with M.G. Mora, M. Peletier, A. Garroni and P. van Meurs.

Lucia Scardia
University of Bath
Dept of Mathematical Sciences
l.scardia@bath.ac.uk

MS73

Wormlike Micellar Solutions: Nonlocality and Shearbanding

Soft materials such as complex fluids may exhibit unusual (non-Newtonian) properties including elastic effects and shear thickening or thinning. Particularly, visco-elastic fluids show fading memory and exhibit nonlocal effects. These fluids often consist of self-assembled transient structures

which can entangle to form a network at the mesoscale. Such transient networks are seen in colloidal solutions, in polymer solutions, and in surfactant solutions. Experiments show that in simple shear rate controlled flow, wormlike micellar solutions (self assembled surfactant solutions) can exhibit inhomogeneous flow patterns namely shear banding. In this talk experimental observations and macroscale and mesoscale modeling and simulations of self-assembling wormlike micellar mixtures will be presented and contrasted. Mathematically the framework is: at the macroscale, a coupled system of nonlinear reaction diffusion equations; at the mesoscale, stochastic differential equations with the topology of the structures tracked. Particular attention is paid to the fluid behavior under changing concentration or temperature in which case the characteristics of the dynamic behavior of the fluid may change considerably.

L. Pamela Cook
University of Delaware
cook@math.udel.edu

Lin Zhou
Mathematics Department, New York City College of Techonology
Brooklyn, NY 11201, USA
lzhou@citytech.cuny.edu

MS73

Energetic Variational Approaches for General Diffusion of Charged Particles.

For the last several years, we had been working on projects related to charge transport in solutions and proteins (ion channels). One of the key ingredients in these studies is the understanding of diffusion and its relations to other effects, such as hydrodynamics, electrostatics and other particle-particle interactions. Due to the non-ideal situations in almost all biological environments, such as the high concentration of charge densities, those conventional theories have to be modified or re-derived. In the talk, I will employ the general framework of energetic variational approaches, especially Onsager's Maximum Dissipation Principles to the problems of generalized diffusion. We will discuss the roles of different stochastic integrations, and the procedures of optimal transport in the context of general linear response theory in statistical physics.

Chun Liu
Department of Mathematics, Penn State University
University Park, PA 16802
liu@math.psu.edu

MS73

On the Memory Terms in the Wave Equations for Poroelastic Materials

This talk focuses on the strategy of approximating the memory terms in the time-domain poroelatic wave equations with Prony's sums. The intrinsic mathematical link between this approximation and the dynamic tortuosity function of the poroelastic media will be explained and the algorithm for obtaining this approximation from permeability data at distinct frequencies will be presented together with some numerical results.

Miao-Jung Y. Ou
University of Delaware, USA
Department of Mathematical Sciences
mou@udel.edu

MS73

A Nonlocal Diffusion Model with Variable Horizons

We study peridynamic models with a spatially varying horizon which mimics a spatial change of scales in nonlocal interactions. We pay particular attention to the issue of convergence in both the nonlocal setting and the local limit. In addition, we also give some applications of our model. 1D interface problems and local-nonlocal coupling problems are also studied.

Yunzhe Tao
Department of Applied Physics and Applied Mathematics
Columbia University
y.tao@columbia.edu

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

MS74

Hydrodynamic Fluctuations of Particle Dynamics Coupled with Continuum

We analyze hydrodynamic fluctuations of hybrid simulation under shear flow. The hybrid simulation consists of a continuum description and a particle dynamics. Moreover, the coupling between the two models is implemented in the framework of the domain decomposition method with overlapping subdomains. In the overlapping region, there is an artificial boundary for each subdomain, respectively. To impose the artificial boundary of the continuum solver, a simple spatial-temporal averaging is performed on the particle simulation ($P \to C$). In the artificial boundary of the particle simulation, four popular strategies of constraint dynamics, that is, the Maxwell buffer, the relaxation dynamics, the least constraint dynamics, and the flux imposition are implemented to achieve a target mean value given by the continuum solver ($C \to P$). Going beyond the mean flows of the hybrid simulations, we investigate the hydrodynamic fluctuations in the subdomain of the particle dynamics. To this end, we calculate the transversal autocorrelation functions of the fluctuating variables in k-space, to evaluate the generation, transportation and dissipation of fluctuations in the presence of a hybrid interface. We show unavoidable contaminations on the fluctuations, due to both the truncation of the subdomain and the constraint dynamics performed in the artificial boundary. Furthermore, we compare the four methods of constraint dynamics and try to reduce the contaminations on fluctuations. Analysis and conclusion in this work are directly applicable to other hybrid simulations of fluid flow with thermal fluctuations.

X Bian
Brown University
xin_bian@brown.edu

MS74

Internal-flow Multiscale Method

Abstract not available

Matthew K. Borg
The University of Edinburgh

matthew.borg@ed.ac.uk

MS74

Equation-Free Approach to Modeling Complex/multiscale Systems

Abstract not available

Minseok Choi
Chemical and Biological Engineering, Princeton University
minseokc@princeton.edu

MS74

Adaptive Resolution Simulation of Supramolecular Water Models

We present adaptive resolution molecular dynamics simulations of aqueous solvents using coarse-grained molecular models that are compatible with the MARTINI force field [J. Zavadlav, M. N. Melo, S. J. Marrink, M. Praprotnik, J. Chem. Phys. **140**, 054114, 2014]. The solvent molecules change their resolution back and forth between the atomistic and coarse-grained representations according to their positions in the system. The difficulties that arise from coupling to a coarse-grained model with a multimolecule mapping could be successfully circumvented by using bundled water models. We discuss the advantages and limitations of this multiscale approach on several examples, e.g., coupling of atomistic water with polarizable [J. Zavadlav, M. N. Melo, S. J. Marrink, M. Praprotnik, J. Chem. Phys. **142**, 244118, 2015] and non-polarizable [J. Zavadlav, M. N. Melo, A. V. Cunha, A. H. de Vries, S. J. Marrink and M. Praprotnik, J. Chem. Theory Comput. **10** 2591, 2014] coarse-grained water models.

Matej Praprotnik
National Institute of Chemistry, Slovenia
praprot@cmm.ki.si

MS75

Morphologies of Semi-Flexible Polymers in Confinement

Microstructure strongly influences the properties of polymeric materials. Prediction of polymer morphology has received considerable attention. Due to computational limitations, most work has focused on flexible chains. Many biological and opto-electronic polymers are better described by a semi-flexible chain. This work utilizes semi-flexible chains in a high performance computing implementation of self consistent field theory to study polymer morphology in confinement. Resulting small particle microstructures will be compared to bulk phases.

David Ackerman, Baskar Ganapathysubramanian
Iowa State University
ackerman@iastate.edu, baskarg@iastate.edu

MS75

Magnetic Field-Induced Pattern Formation in Smectic A Liquid Crystals

We study de Gennes and Chen-Lubensky free energies for smectic A liquid crystals over S^2 valued vector fields to understand the chevron (zigzag) pattern formed in the presence of an applied magnetic field. As the applied field increases, we observe the onset of undulations, which develop into a chevron patterns well above the critical field. Well above the instability threshold, we show via Gamma-convergence that a chevron structure where the director connects two minimum states of the sphere is favored. Numerical simulations illustrating the chevron structures for both models will be presented.

Carlos Garcia-Cervera
Mathematics, UCSB
cgarcia@math.ucsb.edu

Sookyung Joo
Old Dominion University
sjoo@odu.edu

Tiziana Giorgi
Department of Mathematical Sciences
New Mexico State University
tgiorgi@math.nmsu.edu

MS75

Optimal Numerical Approaches to the Stochastic Homogenization of Elliptic Equations and to the Stochastic Drift-Diffusion-Poisson System

In the numerical stochastic homogenization of elliptic problems using the classical results by Kozlov and Yurinskii, it is necessary to choose the size of the finite domain (as well as the boundary conditions), the size of the window for sampling, the FE mesh size, and the number of samples. We present an optimal approach to choosing these parameters based on an error estimate and show results for a Monte-Carlo finite-element implementation. Similar ideas are applied to calculating solutions of the stochastic drift-diffusion-Poisson system using a multi-level Monte-Carlo finite-element discretization.

Clemens Heitzinger, Caroline Geiersbach, Leila Taghizadeh
Vienna University of Technology
clemens.heitzinger@tuwien.ac.at, caroline.geiersbach@gmail.com, leila.taghizadeh@tuwien.ac.at

MS75

Real-Space and Real-Time First-Principle Electronic Structure Calculations Using the FEAST Algorith

We introduce new computational and algorithmic paradigms that can significantly improve the efficiency of existing methodologies used in first principle electronic DFT ground state and TDDFT excited states calculations of complex molecular systems and nanostructures. In particular, we will review the broader impacts of the FEAST eigensolver and present various simulation results with applications ranging from computational electronic spectroscopy of molecules, to plasmonic excitations in carbon-based nanostructures.

Eric Polizzi
University of Massachusetts, Amherst, USA
polizzi@ecs.umass.edu

MS76

Energy Spreading in Strongly Nonlinear Lattices:

From Nonlinear Diffusion to Second Sound

Strongly nonlinear disordered lattices often exhibit chaotic dynamics. I report on two setups for macroscopic relaxation dynamics on top of this chaos. In the first problem, spreading of an initially localized wavepacket on top of vacuum is considered as an effective nonlinear diffusion process. In the second problem, periodic in space perturbations on top of a chaotic state are studied as effective damped oscillating modes.

Arkady Pikovsky
Department of Physics and Astronomy
University of Potsdam, Germany
pikovsky@uni-potsdam.de

MS76

Twist-Stretch Phase Boundaries in Bi-Stable Chains

We consider the dynamics of chains whose springs have a multi-well energy landscape which depends on both twist and stretch. We show that the x-t plane of the dynamics of our chains is analogous to that of a bar capable of twist-stretch phase transitions. Since our numerical integrator for the chain dynamics conserves energy we find that the phase boundaries propagate as if the process is adiabatic and imply a temperature dependent kinetic relation.

Prashant K. Purohit
Mechanical Engineering and Applied Mechanics
University of Pennsylvania
purohit@seas.upenn.edu

MS76

2D Wave Channeling in the Locally Resonant Discrete Structures

Nonlinear wave channeling emerging in the 2D discrete structures incorporating internal rotators is considered. Current study focuses on the analysis of resonant wave manipulation and bifurcation structures of nonstationary regimes. The basic question of possible coexistence of various stationary and non-stationary regimes as well as their local and global bifurcations is addressed. In the limit of low amplitude oscillations we will present the analytical description of the intriguing nonlinear phenomenon of 2D, unidirectional wave entrapment.

Yuli Starosvetsky
Technion, Israel Institute of Technology
staryuli@tx.technion.ac.il

MS76

Solitary Waves in a Lattice with Competing Interactions

We construct a family of solitary waves in a discrete chain with piecewise linear first-neighbor interactions and competing linear second-neighbor interactions. We show that the relative strength of the second-neighbor interactions significantly affects the solution structure and the velocity interval of their existence. Depending on the parameter regime, solutions may have monotone or oscillatory tails and exhibit delocalization or envelope-type structure. Numerical simulations suggest that solutions whose energy increases with velocity are stable.

Anna Vainchtein
University of Pittsburgh
aav@pitt.edu

Lev Truskinovsky
Laboratoire de Mechanique des Solides
Ecole Polytechnique
trusk@lms.polytechnique.fr

MS77

Asymptotic Theory and Experiments on Seismic Metamaterials

Abstract not available

Sebastien Guenneau
Aix-Marseille University
sebastien.guenneau@fresnel.fr

MS77

On the Effect of Dissipation on Anomalous Localized Resonance Phenomena with Applications to Cloaking and Superlensing

In this talk we will present several new developments of our analysis of the anomalous localized resonance phenomena (ALR) and its dependence of loss in the quasistatic and finite frequency regimes. In particular we will show that while the ALR phenomena is very strong in the quasisiatic regime it is extremely weak in the finite frequency regime. Analytical discussion as well as numerical support will reflect our findings in the particular context of an infinite slab of negative permitivity non-magnetic material surrounded in positive but lossy media.

Daniel Onofrei
University of Houston
onofrei@math.uh.edu

Andrew E. Thaler
Institute for Mathematics and its Applications
andythaler05@gmail.com

MS77

Outgoing Wave Conditions in Photonic Crystals and Transmission Properties at Interfaces

We investigate the following transmission problem: a wave travels in free space and hits the boundary of a photonic crystal. Waves are described with Helmholtz equations, in the photonic crystal the Helmholtz equation has x-dependent coefficients. In experiments, a multitude of effects can be observed: (1) perfect reflection. (2) (partial) transmission with (a) positive refraction and (b) negative refraction. (3) creation of localized interface waves. An important step in the analysis of the problem regards the outgoing wave condition in the photonic crystal. The Sommerfeld condition, which is only applicable in free space, must be replaced by an adequate radiation condition. We develop an outgoing wave condition with the help of a Bloch wave expansion. Our radiation condition admits a (weak) uniqueness result which is formulated in terms of the Bloch measure of solutions. Our analytical results confirm known physical principles of the transmission problem: The vertical wave number of the incident wave is a conserved quantity. Together with the frequency condition for the transmitted wave, this condition leads (for appropriate photonic crystals) to the effect of negative refraction

at the interface.

Ben Schweizer
TU Dortmund
Fakultät für Mathematik
ben.schweizer@tu-dortmund.de

MS78

Smectic A Liquid Crystals Under Applied Field in 3D

We study the Landau-de Gennes free energy to describe the undulatory instability in smectic A liquid crystals subjected to magnetic fields. We prove this phenomena by the bifurcation theory to the nonlinear system of Landau-de Gennes model. The bifurcation at the onset of undulation in 3D is not simple. We identify the irreducible representations for natural actions on the functional that take into account the invariances of the problem thus allowing for reducing the bifurcation analysis to a subspace with symmetries. A reduced 2D model provides a qualitative structure of the minimizer. We also perform numerical simulations to illustrate the results of our analysis.

Sookyung Joo
Old Dominion University
sjoo@odu.edu

MS78

The Topology of Defects in Smectics

The order parameter of the smectic liquid crystal phase is the same as that of a superfluid or superconductor, namely a complex phase field. We show that the essential difference in boundary conditions between these systems leads to a markedly different topological structure of the defects. Screw and edge defects can be distinguished topologically. This implies an invariant on an edge dislocation loop so that smectic defects can be topologically linked not unlike defects in ordered systems with non-Abelian fundamental groups.

Randall Kamien
Physics Dept
University of Pennsylvania
kamien@physics.upenn.edu

MS78

Defects in Smectic C Liquid Crystals

If a surface stabilized liquid crystal cell is cooled from the smectic-A to the smectic-C phase its layers thin causing V-shaped (chevron like) defects to form. These sharp bends in turn create an energy barrier that has to be overcome in ferro-electric switching between equilibrium patterns. In the limit as the smectic layer thickness tends to zero, the barrier becomes infinite and ad-hoc terms have been included to overcome it. We examine a gradient flow for a mesoscopic Chen-Lubensky energy $F(\psi, \mathbf{n})$ where the order parameter ψ can vanish. In this model the energy barrier does not diverge as the layer thickness becomes small. The liquid crystal can evolve between equilibrium states in such a way that the layers are allowed to melt and heal, and the cone angle can thin near the chevron tip in the process.

Daniel Phillips
Department of Mathematics, Purdue University
phillips@math.purdue.edu

Lidia Mrad
Purdue University
lmrad@purdue.edu

MS78

Colloidal and Chiral Stabilization of Knotted Nematic Braids

Knotted fields are an emerging research topic relevant to different areas of physics where topology plays a crucial role. Recent realization of knotted nematic disclinations stabilized by colloidal particles raised a challenge of free-standing knots. We have realized free-standing knotted and linked disclination loops in the cholesteric ordering fields, which are confined to spherical droplets with normal boundary condition. In general the stabilization of knots depends on the interplay of the confining geometry, surface anchoring, and intrinsic chirality.

Slobodan umer
Faculty of Mathematics and Physics
University of Ljubljana
slobodan.zumer@fmf.uni-lj.si

MS79

Defect Identification and Analysis Via Topology

Session Code G, Oral A major challenge for atomistic simulation studies of defects in crystalline materials is their automated identification and characterization. Simulations today may contain billions of atoms, and identifying even simple vacancies can be difficult in highly perturbed systems, requiring artificial modification of data through quenching. We introduce an efficient and versatile technique, based on Voronoi cell topology, that enables automated visualization, characterization, and analysis of complex defect structure, even at temperatures near melting.

Emanuel A. Lazar
University of Pennsylvania
Department of Materials Science and Engineering
mlazar@seas.upenn.edu

Jian Han, David J. Srolovitz
University of Pennsylvania
jianhan@seas.upenn.edu, srol@seas.upenn.edu

MS79

Variational Models for Crystal Image Analysis

Computer-assisted or automated analysis of atomic-scale resolution image for polycrystalline materials has important applications in characterizing and understanding material micro-structure. In this talk, we will discuss some recent progress in crystal image analysis using 2D synchrosqueezed transforms combined with variational approaches.

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

Benedikt Wirth
Universität Münster
benedikt.wirth@uni-muenster.de

Haizhao Yang
Duke University
Math Dept, Duke University
haizhao@math.duke.edu

MS79

Energy Scaling and Asymptotic Properties of Step Bunching in Epitaxial Growth with Elasticity Effects

In epitaxial growth on vicinal surfaces, elasticity effects which give rise to step bunching instability and some self-organization phenomenon are widely believed to be important in the fabrication of nanostructures. However, due to the nonlocal effects and the interaction between different length scales, difficulties appear in the modelling and analysis of these growth process. In this paper, we study a discrete model for epitaxial growth with elasticity. We rigorously prove the minimum energy scaling law, the appearance of one bunch structure and provide sharp bounds for the bunch size as well as the slope of the optimal profile.

Tao Luo, Yang Xiang
Hong Kong University of Science and Technology
tluoaa@ust.hk, maxiang@ust.hk

Aaron Nung Kwan Yip
Purdue University
Department of Mathematics
yip@math.purdue.edu

MS79

A New Proof of Convergence to Motion by Mean Curvature for the Bence-Merriman-Osher Algorithm

We provide a new proof of the convergence to motion by mean curvature for the classical thresholding scheme initiated by Bence, Merriman, Osher in 1992. The current proof is elementary and does not require the convolution kernel to be positive. It thus has the potential to be generalized to higher flows for which maximum principle is not applicable. The idea is based on the construction of suitable ansatz and the regularity property of the curvature motion.

Drew Swartz
Booz Allen Hamilton
Washington D. C.
drew.e.swartz@gmail.com

Aaron Yip
Purdue University
yipn@purdue.edu

MS80

Self-Assembled Nanoscale Patterns Produced by Ion Bombardment of Solid Surfaces

When a solid surface is bombarded with a broad, obliquely-incident beam of noble gas ions, nanoscale surface ripples often develop. We have advanced a theory that explains why these ripples ultimately take on a terraced form for high angles of incidence. In our theory, the regions where the surface slope changes precipitously are undercompressive shocks. A related theory explains the results of recent experiments in which elemental materials were bombarded with beams of non-volatile ions, yielding hexagonal arrays of nanoholes for normal-incidence bombardment and disordered herringbone patterns for oblique incidence.

R. Mark Bradley
Department of Physics
Colorado State University
bradley@lamar.colostate.edu

MS80

Optimal Estimates on Contact Line Propagation for the Thin-Film Equation

Consider a thin viscous droplet spreading on a solid surface; the evolution of the droplet is then approximated by the thin-film equation. We present a method for the derivation of lower bounds on contact line propagation for the thin-film equation. In particular, we obtain sufficient conditions for instantaneous forward motion of the contact line as well as lower bounds on asymptotic propagation rates. These results are based on new monotonicity formulas for the thin-film equation and constitute the first mathematical lower bounds on free boundary propagation for any higher-order degenerate parabolic equation.

Julian Fischer
Max Planck Institute for Mathematics in the Sciences, Leipzig
julian.fischer@mis.mpg.de

MS80

Stability and Dewetting of Metal Thin Films on Semiconductor Substrates: Clarifying the Role of Quantum Size Effect

Zhang *et al.* (PRL 80, 5381 (1998)) demonstrated that the so-called quantum size effect (QSE) is prominent in ultra-thin metal films (thickness < 30 ML) on semiconductor substrates. We consider a morphological instability of a planar surface ([111], [011], or [001]) of such film in a parameter space formed by three major effects, e.g. the QSE, surface energy anisotropy, and surface stress. The analysis is based on the surface diffusion equation, where the effects are cast as the functions of the film thickness. The formulation includes the oscillations of the QSE component of the surface energy with thickness, and the impacts of these oscillations on a film stability are determined.

Mikhail V. Khenner
Western Kentucky University
mikhail.khenner@wku.edu

MS80

External-Field-Driven Stabilization and Patterning of Materials Surfaces

Based on atomistically informed continuum-scale computational models in conjunction with linear and nonlinear stability analyses, we address problems of surface morphological instabilities in stressed elastic solid material systems, develop surface stabilization strategies by exploiting the action of externally applied electric fields and thermal gradients, and explore complex patterns that may emerge from stress-induced instabilities. We also introduce the current-driven dynamics of single-layer islands on conducting substrate surfaces as a directed assembly strategy for surface nanopatterning.

Dimitrios Maroudas

University of Massachusetts, Amherst
maroudas@ecs.umass.edu

MS81

Time Domain Inverse Problem for Maxwell's Equations in Microstructured Media

Homogenization of Maxwell's equations for a multiscale dispersive medium results in time-convolution equations with a memory kernel. We relate this kernel to the spectral measure of the problem on the microscale and use it to derive information about the geometry of the finely structured medium.

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

Niklas Wellander
Swedish Defence Research Agency, FOI
niklas.wellander@foi.se

Dali Zhang
University of Calgary
Department of Mathematics
dlzhang@math.ucalgary.ca

MS81

Inverse Problems for Sea Ice

Monitoring the internal state of sea ice, and its response to climate change, involves inverse problems which are of broad interest in remote sensing applications. I will discuss inverse homogenization problems for composite materials such as sea ice, as well as related problems on larger scales for data on ice pack dynamics.

Kenneth M. Golden
University of Utah
Department of Mathematics
golden@math.utah.edu

MS81

Homogenization of a Transmission Problem

Abstract not available

Shari Moskow
Drexel University
Department of Mathematics
moskow@math.drexel.edu

MS81

Exact Determination of the Volume of An Inclusion in a Body with Constant Shear Modulus

We derive an exact formula for the volume fraction of an inclusion in a body when the inclusion and the body are linearly elastic materials with the same shear modulus. Our formula depends on an appropriate measurement of the displacement and traction around the boundary of the body. In particular, the boundary conditions around the boundary of the body must be such that they mimic the body being placed in an infinite medium with an appropriate displacement applied at infinity.

Andrew E. Thaler
Institute for Mathematics and its Applications
andythaler05@gmail.com

Graeme W. Milton
University of Utah
Department of Mathematics
milton@math.utah.edu

MS82

Temperature and Thermal Transport in Defect Kinetics: Thermomechanical Analysis of Phase Transformations in an Atomic Chain

Analysis in the literature on a phase-transforming chain of atoms finds that a one-parameter family of kinetic relations emerges by considering steadily-moving phase boundaries as traveling waves. We propose and numerically test the hypothesis that this one-parameter family represents a temperature- and heat flux- dependent kinetic relation in the framework of continuum thermoelasticity. From this perspective, the "no-radiation" selection criterion that is used to pick a particular solution from this family in fact corresponds to a statement about the heat flux and temperature fields in the vicinity of the moving defect in a macroscopic body.

Kaushik Dayal
Carnegie Mellon University
kaushik@cmu.edu

MS82

Averaging Evolving Dislocation Systems with De Rham Currents

De Rham currents are a generalization of Schwartz distributions which establish a duality of differential forms and submanifolds. Dislocations are line-like crystal defects mediating plasticity in crystals. Considering dislocations as moving oriented curves we employ (vector valued) de Rham currents to obtain averaged descriptions of dislocations and plasticity in terms of alignment tensors and their evolution equations. Challenges for averaging in the case of large deformations will be discussed.

Thomas Hochrainer
University of Bremen
Bremer Institut für Strukturmechanik und Produktionsanlagen
hochrain@uni-bremen.de

MS82

Entropy Production and Microstructure Evolution in Materials

The modeling of continuum dissipative evolution equations remains a challenge and is currently based on phenomenological constitutive relations (e.g., Fouriers law for heat transfer). In this talk we present some connections between the geometry of dissipative evolution equations, the principle of maximum entropy production, large deviation principles for stochastically augmented evolution equations and fluctuation-dissipation relations. Its application to the evolution of microstructures in materials will be discussed.

Celia Reina
University of Pennsylvania
Penn Institute for Computational Science

creina@seas.upenn.edu

Johannes Zimmer
University of Bath
j.zimmer@bath.ac.uk

MS83

Material Interfaces and Boundary Conditions in Nonlocal Diffusion.

Convergence of a nonlocal diffusion model inside heterogeneous media in the limit of vanishing nonlocality is analyzed. The associated integral operator converges to its local counterpart in the limit of vanishing nonlocality, when the material diffusivity is sufficiently differentiable. However, when the material diffusivity has discontinuities, as in multiphase composites, the nonlocal diffusion operator diverges, in the local limit, at material interfaces. Nonlocal interface jump conditions are introduced which generalize local interface conditions. A nonlocal diffusion model for composite media that is locally consistent with classical diffusion in composites is presented.

Bacim Alali
Mathematics Department
University of Utah
bacimalali@math.ksu.edu

MS83

Multiscale Finite Elements for Nonlocal Materials Models and Local-Nonlocal Coupling.

The problem of computing quantum-accurate design-scale solutions to mechanics problems is rich with applications and serves as the background to modern multiscale science research. The peridynamic model for continuum mechanics provides an advantage in this endeavor, as the basic equations are valid at a wide range of scales limiting from the classical PDE at the design scale to the scale of molecular dynamics. In this work we focus on the development of multiscale finite element methods for the peridynamic model as a step towards computationally tractable, high-fidelity multiscale simulations.

Timothy Costa
Oregon State University
costat@math.oregonstate.edu

Stephen D. Bond
Computer Science
University of Illinois at Urbana-Champaign
sdbond@sandia.gov

David Littlewood
Sandia National Laboratories
djlittl@sandia.gov

MS83

A Trace Theorem for a Class of Nonlocal Energy Spaces

It is a classical result on Sobolev spaces that any H^1 function has a well-defined $H^{1/2}$ trace on the boundary of a domain with enough smoothness. In this work, we present a nonlocal extension of such a trace theorem in a new function space which contains H^1 as a subspace. This new space is associated with a nonlocal energy norm which is characterized by a nonlocal interaction kernel defined heterogeneously. We show that the $H^{1/2}$ norm of the trace on the boundary is controlled by the nonlocal energy norm. This result is novel in the sense that the boundary trace is attained without imposing regularity of the function in the interior of the domain. The result has various applications. In particular, it provides a theoretical foundation to the coupling of nonlocal and local models.

Xiaochuan Tian, Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
xt2156@columbia.edu, qd2125@columbia.edu

MS83

Mathematical and Numerical Analysis for Nonlocal Parabolic Equations

We consider an initial/boundary value problem for nonlocal parabolic equations involving a nonlocal derivative in time. We study the well-posedness, spatial regularity pickup and also the localization of the model. Further, we present some preliminary results on numerical analysis. We develop an semidiscrete scheme using standard Galerkin finite element method, and derive the error estimates which are expressed in terms of the smoothness of the initial or the source data. Extensive numerical results are presented to illustrate our theoretical findings.

Zhi Zhou
Columbia University
zhouzhi19880125@gmail.com

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

Jiang Yang
Columbia University
jyanghkbu@gmail.com

MS84

Hybrid Multiscale Finite Volume Method for Advection-Diffusion-Reaction Equations

We present a hybrid scheme for the coupling of macro and microscale advection-diffusion models for reactive contaminant transport in fractured and porous media. The Multiscale Finite Volume (MsFV) method is employed to approximate the microscale field in terms of local functions and global degrees of freedom. The MsFV global problem is then coupled with the macroscopic model. We propose a split local-global timestepping scheme for integrating macro and microscale problems using different timesteps.

David A. Barajas-Solano
Pacific Northwest National Lab
david.barajas-solano@pnnl.gov

Alexander Tartakovsky
Pacific Northwest National Laboratory
alexandre.tartakovsky@pnnl.gov

MS84

Transport in Porous Electrodes Using a Multiscale

Modeling Approach

Abstract not available

W. Pan
Pacific Northwest National Laboratory
wenxiao.pan@pnnl.gov

MS84

Parameter Inference Via Multi-Fidelity Information Fusion

We present a computational framework for model inversion based on multi-fidelity information fusion and Bayesian optimization. The proposed methodology targets the accurate construction of response surfaces in parameter space, and the efficient pursuit to identify global optima while keeping the number of expensive function evaluations at a minimum. We train families of correlated surrogates on available data using Gaussian processes and auto-regressive stochastic schemes, and exploit the resulting predictive posterior distributions within a Bayesian optimization setting. The effectiveness of the proposed framework is tested on a parameter estimation problem involving the calibration of outflow boundary conditions in blood flow simulations using multi-fidelity realizations of one- and three-dimensional models. This work received support from DARPA grant HR0011-14-1-0060.

Paris Perdikaris
Massachusetts Institute of Technology
parisp@mit.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS84

Time-Scale Bridging in Coagulation Cascade and Blood Clotting Simulations Through a Multifidelity Algorithm

The process of clot formation and growth at a site on a blood vessel wall involve a number of multiscale simultaneous processes. Normally, the physiological values of reaction rates result in a clotting process of the order of minutes making the simulations prohibitively long. We propose a multifidelity technique in order to facilitate acceleration in time. We also perform multiscale simulations of the clotting process in a venule and in a realistic geometry of aortic dissection and aneurysm.

Alireza Yazdani
Brown University
alireza_yazdani@brown.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS85

Title Not Available

Abstract not available

Nawaf Bou-Rabee
Mathematics
Rutgers Camden
nawaf.bourabee@rutgers.edu

MS85

Unpacking the Thermodynamics of Small Molecule Adsorption on Nanomaterial Surfaces

Free-energy calculation techniques applied to molecular dynamics simulation can yield accurate predictions of the thermodynamics and kinetics of interactions at nanomaterialsolution interfaces, accelerating the design and optimization of nanomaterials for applications such as drug delivery and contaminant sequestration. However, such predictions require reliable models of nanomaterial surfaces as well as accurate descriptions of their interactions with relevant solutes. Here I show that existing models give excellent agreement with experimental results (correlation = 0.9) for the relative adsorption affinities of a set of about 30 small aromatic molecules on naked and hydroxylated carbon nanotubes. However, the absolute values of the equilibrium constants differ by as much as an order of magnitude, and there are some signs of relative imbalances, for instance, between alkyl-substituted benzenes and phenolics. In an attempt to identify the source of such imbalances, we have determined the contributions of different physical effectsincluding desolvation, conformational entropy, hydrogen bonding, and van der Waals and electrostatic energiesto the calculated equilibrium constants. I will describe how isolating these contributions elucidates the physical details of adsorbatesurface interaction and can help to improve the force fields and models.

Jeffrey Comer
Kansas State
jeffcomer@ksu.edu

Ran Chen, Horacio Poblete, Ariela Vergara-Jaque, Jim Riviere
Kansas State University
ranchen19@gmail.com, hpoblete@ksu.edu, avergara@ksu.edu, jriviere@vet.k-state.edu

MS85

Information Theoretic Fitting for Coarse-Grained Molecular Dynamics

A wide range of coarse graining techniques for molecular systems exist to reduce the vast state space and timescales inherent in many systems of interest. One class of approaches map the continuous configuration space of a dynamics onto a discrete set of configurations, and construct an approximation of the resulting coarse-grained process. We consider coarse-graining of stochastic trajectories and using information theory techniques to fit mesoscale models that capture averaged behavior as well as short-term memory effects of the process.

Matthew Dobson
University of Massachusetts Amherst
dobson@math.umass.edu

MS85

Stochastic Processes and Diffusive Molecular Dynamics

Diffusive Molecular Dynamics (DMD) is a novel approach to problems in molecular dynamics that aims to reach the diffusive time scale of milliseconds and beyond. To accom-

plish this, DMD averages out the vibrational time scale of femtoseconds and evolves probability densities at atomistic sites. This requires the approximation of a probability distribution in an extended state space by a synthetic approximate distribution, which can easily be sampled. The mean occupancy at the atomic sites are then evolved according to a system of coupled ODEs, under a so-called Master Equation, but no underlying stochastic process is given in the current formulation. In this work, we propose and examine a stochastic process which gives rise to similar dynamics as DMD. This primitive model also offers a way to connect DMD to a more traditional MD models.

Brittan A. Farmer
Department of Mathematics
University of Michigan
farbritt@umich.edu

Mitchell Luskin
School of Mathematics
University of Minnesota
luskin@math.umn.edu

Petr Plechac
University of Delaware
Department of Mathematical Sciences
plechac@math.udel.edu

Gideon Simpson
Department of Mathematics
Drexel University
simpson@math.drexel.edu

David J. Srolovitz
University of Pennsylvania
srol@seas.upenn.edu

MS85

Analysis and Optimization of Stratified Sampling

Stratified sampling methods compute averages over a target distribuion by partitioning the sample space into subregions, sampling conditional distributions confined to the subregions, and computing averages over the target distribution from the conditional averages. Such methods may be used to compute both averages with respect to the ergodic measure of a process and also dynamical quantities, such as reaction rates, of interest in molecular simulation. We analyze the benefits of stratified sampling, and we discuss some techniques for optimizing the parameters involved in the method.

Brian Van Koten
University of Chicago
bvankoten@gmail.com

Aaron Dinner
James Franck Institute
University of Chicago
dinner@uchicago.edu

Jeremy Tempkin, Erik Thiede
Chemistry
The University of Chicago
jtempkin@uchicago.edu, thiede@uchicago.edu

Jonathan Weare
University of Chicago
Department of Statistics and the James Franck Institute
weare@uchicago.edu

MS86

Asymptotic Formulas for Lattice Waves in the High-Energy Limit

Nonlinear lattice waves play a prominent role in many branches of materials science and can be regarded as the fundamental modes of spatially discrete systems with dispersive and nonlinear interactions. The corresponding mathematical theory, however, is rather complicate since the underlying equations are not ODEs but involve advance and delay terms. In this talk we study the high-energy limit of FPU-type chains and derive asymptotic ODEs which determine both the shape and the speed of the corresponding lattice waves up to high accuracy. The resulting formulas are almost explicit and provide a good starting point to investigate further dynamical properties such as linear or nonlinear stability.

Michael Herrmann
University of Muenster
michael.herrmann@uni-muenster.de

Karsten Matthies
Department of Mathematical Sciences
University of Bath
K.Matthies@maths.bath.ac.uk

MS86

Traveling Waves in Lattices with Obstacles

We consider scalar, bistable lattice differential equations on rectangular lattices in two space dimensions. We show that under certain natural conditions that wave like solutions exist when obstacles (characterized by "holes') are present in the lattice. The results here generalize to spatially discrete problems, the results on propagation through obstacles for partial differential equations obtained by Berestycki, Hamel and Matano. The analysis hinges upon development of sub and supersolutions for this class of higher space dimension lattice differential equations and on a generalization of a classical result of Aronson and Weinberger on the spreading of localized disturbances.

Aaron Hoffman
Franklin W. Olin College of Engineering
aaron.hoffman@olin.edu

Hermen Jan Hupkes
University of Leiden
Mathematical Institute
hhupkes@math.leidenuniv.nl

Erik Van Vleck
Department of Mathematics
University of Kansas
evanvleck@math.ku.edu

MS86

Solitary Waves in the Burridge-Knopoff Model

The Burridge-Knopoff model describes a chain of blocks connected by springs and pulled over a surface. The blocks are subject to a nonlinear velocity-dependent friction force which is non-monotonic and induces excitability. We introduce a simplified piecewise linear friction law (reminiscent of the McKean nonlinearity in spiking neuron models)

which allows us to prove the existence of large amplitude solitary waves and study their qualitative properties.

Guillaume James
INRIA - Rhône Alpes
guillaume.james@inria.fr

Jose Eduardo Morales Morales
INRIA Rhone Alpes
jose-eduardo.morales-morales@inria.fr

Arnaud Tonnelier
INRIA - Rhône Alpes
arnaud.tonnelier@inria.fr

MS86

KdV Dynamics and Traveling Waves in Polyatomic FPU

Using homogenization theory, we can derive and justify a Korteweg-deVries limit for a polyatomic Fermi-Pasta-Ulam lattice problem under the assumption that the material parameters vary periodically. While the KdV approximation predicts the existence of solutions which look like solitary waves for long times, it does not guarantee that such solutions remain coherent forever. We discuss recent results on the global in time existence of "generalized solitary waves" in diatomic FPU lattices.

Timothy Faver
Drexel University
tef36@drexel.edu

Shari Moskow
Drexel University
Department of Mathematics
moskow@math.drexel.edu

Ronald Perline
Drexel University
rperline@math.drexel.edu

Yuli Starosvetsky
Technion, Israel Institute of Technology
staryuli@tx.technion.ac.il

Anna Vainchtein
Department of Mathematics
University of Pittsburgh
aav4@pitt.edu

Doug Wright
Drexel University
Mathematics
jdoug@math.drexel.edu

MS87

Parity-Time Symmetric Metasurfaces

We discuss the unusual wave interactions with pairs of metasurfaces characterized by balanced loss and gain, which are invariant under s parity-time symmetry transformation. Their features provide a fertile ground to realize invisibility cloaks that overcome the limitations of conventional passive cloaks, shadow-less sensors, and negative-index slabs, leading to aberration-free imaging devices. Stability and bandwidth considerations will be discussed during the talk.

Andrea Alu
Department of Electrical and Computer Engineering
University of Texas at Austin
alu@mail.utexas.edu

MS87

Numerical Simulation of Wave Propagation in Advanced Materials and Structures

The response of many materials of engineering interest to external loading is influenced by their microstructure. The components of such a microstructure may have different material properties, resulting in an enormous complexity in the response of a material. Computation of high strain rate processes in real materials and structures with necessary efficiency and accuracy is an important task. Results of numerical simulations by means of a thermodynamically consistent algorithm are demonstrated on examples of wave propagation. As a preliminary study to more complex situations of interest in small-scale technology, this study envisages the propagation properties of elastic waves in one-spatial dimension when some of the properties may vary suddenly in space or in time. We are interested in so-called dynamic materials (DM). Dynamic materials are artificially constructed structures (like metamaterials) which may vary their characteristic properties in space or in time, or both, by an appropriate arrangement or control. These controlled changes in time can be provided by the application of an external (non-mechanical) field, or through a phase transition. Such materials exhibit very unusual behavior.

Mihhail Berezovski
Institute of Cybernetics at Tallinn University of Technology
mihhail.berezovski@gmail.com

MS87

Imaging of Chiral Gratings in Inverse Electromagnetic Scattering

We consider the electromagnetic inverse scattering problem for the Drude-Born-Fedorov model for periodic chiral structures known as chiral gratings both in two and three dimensions. The Factorization method is studied as an analytical as well as a numerical tool for solving this inverse problem. The method constructs a simple criterion for completely characterizing shape of the periodic scatterer which leads to a uniqueness result and a fast imaging algorithm. The required data consists of certain components of Rayleigh sequences of (measured) scattered fields caused by plane incident electromagnetic waves. We propose in this electromagnetic plane wave setting a rigorous analysis for the Factorization method. Numerical examples in two and three dimensions are also presented for showing the efficiency of the method.

Dinh Liem Nguyen
University of Michigan, Ann Arbor
dlnguyen@umich.edu

MS87

Perfectly Matched Layers for Dispersive Media and Application to Time-Domain Simulations in Metamaterials

The standard Perfectly Matched Layers (PMLs) are unsta-

ble for Negative Index Metamaterials (NIMs). We will provide a stability analysis of more general PMLs for a large class of dispersive media that includes NIMs. It will allow us to construct new stable PMLs for NIMs. We then use them to highlight some interesting phenomena concerning the long-time behaviour of the solution of a transmission problem in the time domain between a dielectric and a NIM.

Valentin Vinoles
ENSTA Paris Tech University
valentin.vinoles@ensta-paristech.fr

Eliane Bécache, Patrick Joly
POems (UMR 7231 CNRS-INRIA-ENSTA)
eliane.becache@inria.fr, patrick.joly@inria.fr

MS88

Sharp-edged Colloidal Particles: Kinked Nematic Disclinations and Shape-tunable Assembly Behavior

For cylindrical and cubical homeotropic colloidal particles in nematic liquid crystals, companion defect configurations and effective interactions are strikingly different than in the well-studied case of spherical colloidal particles. We show, using Landau-de Gennes numerical modeling, that disclinations pin at portions of the colloidal particles' sharp edges. This leads to kinked disclination lines with interesting multistable configurations, and to shape-tunable oblique particle alignment relative to the far-field nematic director, as confirmed in accompanying experiment.

Daniel Beller
Harvard University
dbeller@seas.harvard.edu

Mohamed Gharbi
McGill University
magharbi83@gmail.com

Iris Liu
University of Pennsylvania
liubi@seas.upenn.edu

MS88

Minimizers of the Landau-de Gennes Energy Around a Spherical Colloid Particle

We consider energy minimizing configurations of a nematic liquid crystal around a spherical colloid particle, in the context of the Landau-de Gennes model. The nematic is assumed to occupy the exterior of a ball B_{r_0}, and satisfy homeotropic weak anchoring at the surface of the colloid and approach a uniform uniaxial state as $|x| \to \infty$. We study the minimizers in two different limiting regimes: for balls which are small $r_0 \ll L^{\frac{1}{2}}$ compared to the characteristic length scale $L^{\frac{1}{2}}$, and for large balls, $r_0 \gg L^{\frac{1}{2}}$. The relationship between the radius and the anchoring strength W is also relevant. For small balls we obtain a limiting quadrupolar configuration, with a "Saturn ring' defect for relatively strong anchoring, corresponding to an exchange of eigenvalues of the Q-tensor. In the limit of very large balls we obtain an axisymmetric minimizer of the Oseen–Frank energy, and a dipole configuration with exactly one point defect is obtained.

Lia Bronsard, Stan Alama
McMaster University
Department of Mathematics and Statistics
bronsard@mcmaster.ca, alama@mcmaster.ca

Lamy Xavier
Max-Planck-Institute for Mathematics in the Sciences
Leipzig
xavierlamy@gmail.com

MS88

Magnetic Nematic Colloids

A colloidal suspension of ferromagnetic nano-particles of barium hexaferrite in a liquid crystal, quenched into the nematic phase, exhibits true ferromagnetic properties1. Cooling in the absence of the magnetic field produces a polydomain sample with two opposite states of magnetization parallel to the nematic ordering. After cooling in magnetic field a monodomain sample is obtained. Magnetization can be switched by domain wall movement in reversed field. The existence of this unique ferromagnetic dipolar fluid is due to interplay of nematic elastic interaction that crucially depends on the shape of the particles and magnetic dipolar interaction. Optical and magnetic response to magnetic and electric field is well described by a simple free energy.

Martin Copic
University of Ljubliana
martin.copic@fmf.uni-lj.si

MS88

Optimizing Inclusions in Nematic Domains with the Ericksen Model

We present a phase-field method coupled to the Ericksen model for equilibrium configurations of liquid crystals with variable degree of orientation. The phase-field accounts for the presence of "holes" in the domain (i.e. inclusions). Our method is based on a finite element formulation and is able to handle the elliptic degeneracy present in the Ericksen model. Simulations in 2-D and 3-D are presented to illustrate the method.

Shawn W. Walker
Louisiana State University
Department of Mathematics and CCT
walker@math.lsu.edu

MS89

Dislocation Climb in Discrete Dislocation Dynamics

We derive a Green's function formulation for the climb of curved dislocations and multiple dislocations in three-dimensions. In this new formulation, the dislocation climb velocity is determined from the Peach-Koehler force on dislocations through vacancy diffusion in a non-local manner. We also present a numerical discretization method of this Green's function formulation appropriate for implementation in discrete dislocation dynamics simulations.

Yejun Gu, Yang Xiang
Hong Kong University of Science and Technology
yguab@ust.hk, maxiang@ust.hk

David J. Srolovitz
University of Pennsylvania

srol@seas.upenn.edu

MS89

Second Kind Integral Equation Formulation for Dislocation Climbs in Two Dimensions

We present a second kind integral equation (SKIE) formulation for the study of dislocation dynamics in two dimensions. Previously the best method for this problem which captures the correct physics uses Green's function directly and is equivalent to a first kind integral equation formulation. Our SKIE formulation is efficient, robust and well conditioned with unknowns only on material interfaces. The boundary integral equations (BIE) are then discretized via the quadrature by expansion (QBX) and solved with the fast multipole method (FMM) and GMRES. The recently developed QBX scheme is a high order quadrature for the evaluation of (weakly) singular, nearly singular, and hypersingular integrals and can be naturally incorporated into the FMM. The FMM accelerated QBX method provides a high order integrated scheme with linear complexity for the discretization, solving, and evaluation phases of BIEs. The performance of the overall scheme is illustrated via several numerical examples.

Shidong Jiang
Department of Mathematical Sciences
New Jersey Institute of Technology
shidong.jiang@njit.edu

Manas N. Rachh
Courant Institute
NYU
manas.rachh@yale.edu

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

MS89

Elastic Interactions and Rare Events in Irradiated Materials

In standard mean-field methods for modelling microstructural evolution, defects are allowed to *react* via diffusion limited capture or splitting, but not *interact*: their chemical potentials are independent of the concentration of other defects. But recent experimental work and multiscale simulations have begun to establish the importance of long-range interactions between irradiation-induced defects. Using in-situ TEM, Yi et al. [Yi et al EPL, 110 (2015) 36001] were able to directly observe multiple large (several nanometre diameter) defects produced in individual cascade events in ultra-high-purity W foil. As the elastic energy between dislocation loops scales with the product of their areas and inversely with the cube of the separation between their centres, the elastic energy inferred in these cascades must be sufficient to bias microstructural evolution even for the smallest observable defects. In this work I will show how experimental observations of UHP W foil irradiated at cryogenic (30K) to high temperatures (1000K) are only reproduced by a simple object kinetic Monte Carlo model if elastic interactions are taken into account. We will explore the significance of rare events, the importance of using the correct set of starting conditions, and reveal some efficient numerical tricks for evolving defects flickering at picosecond timescales out to observable times of seconds and beyond.

Daniel Mason
Culham Centre For Fusion Energy
daniel.mason@ukaea.uk

Xiaoou Yi
Oxford University
xiaoou.yi@materials.ox.ac.uk

Andrea Sand
University of Helsinki
andrea.sand@helsinki.fi

Mark Kirk
Argonne National Laboratory
kirk@anl.gov

Sergei Dudarev
University of Oxford and Culham Centre for Fusion Energy, UK
Sergei.Dudarev@ccfe.ac.uk

MS89

An Efficient Level-let Model for Grain Growth Customized for Supercomputers

We present a new implementation strategy for a level-set model for 2- and 3D grain growth, which allows for an optimal utilization of the model in parallel computers. The strategy is based on the decomposition of the microstructure into the smallest possible objects i.e. the grains. This results in a very flexible decomposition of the original microstructure that permits the distribution of the computational tasks. The numerical scheme turns out to be highly memory-efficient and shows strong scaling on shared memory architecture up to 128 cores. The model is capable of considering the full complexity of the grain boundary structure including the properties of triple junctions, which are microstructural features of high relevance for nanocrystalline materials. To demonstrate the accuracy of the model and benchmark its performance, the bulging behavior of subgrains at orientation bands was studied. By utilization of data analytics, it was possible to determine the crystallographic conditions that are necessary for the growth of these grains.

Christian Mieen
Institute of Physical Metallurgy and Metal Physics
RWTH Aachen University
miessen@imm.rwth-aachen.de

Nikola Velinov, Markus Kühbach, Luis-Antonio Barrales-Mora, Günter Gottstein
Institute of Physical Metallurgy and Metal Physics
RWTH Aach
nikola.velinov@rwth-aachen.de, kuehbach@imm.rwth-aachen.de, lbarrales@imm.rwth-aachen.de, gottstein@imm.rwth-aachen.de

MS90

The Formation and Stability of Heteroepitaxial Nanorings

Self-assembled nanorings have recently been identified in a number of strained material systems. The energetics and kinetics of the formation of these structures is investigated. Under some circumstances these rings have been observed

to break up into quantum dots. The stability of these nanorings is modelled. A region of stability is predicted below a critical radius. The predictions of the model are shown to be consistent with experimental results.

Simon Gill
University of Leicester
spg3@leicester.ac.uk

MS90

Virtually Defect Free Nanoscale Ripples Produced by Ion Bombardment of Rotating Solid Surfaces

Bombardment of a solid surface with a broad, obliquely-incident ion beam frequently produces nanoscale surface ripples. These ripples are well described by the Kuramoto-Sivashinsky (KS) equation, which produces spatiotemporal chaos. We show that a modification of the experimental setup results in a surface described by the KS equation with coefficients that vary periodically in time, and that this temporally periodic driving can suppress the spatiotemporal chaos and yield near perfect spatial periodicity.

Matt P. Harrison, Mark Bradley
Colorado State University
mattharrison2718@gmail.com,
mark.bradley@colostate.edu

MS90

Growth in Confined Environments

We discuss the dynamics of growing interfaces in confined environments, and the relevance of this process in geology. We present a model which includes the competition of diffusion and hydrodynamics to transport mass to the interface in confinement. We also explore the force of crystallization exerted by the growing crystal on the substrate.

Oliver Pierre-Louis
Université Claude Bernard Lyon 1
olivier.pierre-louis@univ-lyon1.fr

Luca Gagliardi
UCBL Lyon 1
luca.gagliardi@ens-lyon.fr

MS90

Corner Wetting During the Vapor-Liquid-Solid Growth of Faceted Nanowires

We consider the corner wetting of liquid drops in the context of vapor-liquid-solid growth of nanowires. Specifically, we construct numerical solutions for the equilibrium shape of a liquid drop on top of a faceted nanowire by solving the Laplace-Young equation with a free boundary determined by mixed boundary conditions. We determine the near-singular scaling behavior near corners of the nanowire and determine the drop shape in terms of the Young contact angle and drop volume.

Brian J. Spencer
University at Buffalo
Department of Mathematics
spencerb@buffalo.edu

MS91

Kirchhoff Migration without Phases

Scatterers in a homogeneous medium can be imaged using the Kirchhoff migration functional. This functional generally requires full waveform measurements of the scattered field and thus intensity (i.e. phaseless) measurements are insufficient to image with. However, if the scattered field is small compared to the probing field, we can solve a simple least-squares problem to recover the projection (on a known subspace) of the full waveform scattered field from intensity data. For high frequencies, this projection gives a Kirchhoff image asymptotically identical to the Kirchhoff image obtained from full waveform data. We can also use this method when the illuminating wavefields are stochastic and we measure autocorrelations at receivers.

Patrick Bardsley
University of Utah
bardsley@math.utah.edu

MS91

Imaging Polarizable Dipoles

We consider the problem of imaging electric dipoles in a homogeneous medium from measurements of all three components of the electric field at an array of receivers. We show that an electromagnetic version of Kirchhoff migration can be used to recover the position and orientation of the dipoles. We prove that the resolution estimates for the position are identical as in the acoustic case and provide error estimates for the dipole orientation.

Maxence Cassier, Fernando Guevara Vasquez
University of Utah
cassier@math.utah.edu, fguevara@math.utah.edu

MS91

Optimal Design for Reactive-Diffusion in Materials

The application of materials for energy conversion hinges on the ability to enable transport of multiple species through different phases and chemical reactions at selected interfaces. We consider the optimal design of diffusive material with reaction in the variational setting using an Allen-Cahn energy contribution. The relation between the relaxed problem arising in the sharp-interface limit and the homogenized behavior will be discussed as well as numerical results for a 2-dimensional problem.

Lincoln Collins
California Institute of Technology
lcollins@caltech.edu

Kaushik Bhattacharya
Howell N. Tyson Sr. Professor of Mechanics
California Institute of Technology
bhatta@caltech.edu

MS91

Inverse Scattering Problems without the Phase Information

The phaseless inverse scattering problem arises in imaging of nano-structures. One uses light source whose wavelength

is in the range $[0.078, 0.126]\mu m$ to illuminate those structures and collects the intensity of the complex scattering field on the sphere outside them. Due to the smallness of the wavelength, measuring the phase of the scattering field is impossible. In this talk, we will show an effective method to reconstruct the lost phase and then provide the solutions for the phaseless inverse scattering problems. This is a joint work with Michael Klibanov and Kejia Pan.

Hoang Loc Nguyen
UNC Charlotte
loc.nguyen@epfl.ch

Michael V. Klibanov
University of North Carolina at Charlotte
Department of Mathematics
mklibanv@email.uncc.edu

Kejia Pan
School of Mathematics and Statistics
Central South University, China
pankejia@hotmail.com

MS92

An Algorithmic Consistent Two-scale Homogenization Scheme for the Characterization of Micro-heterogeneous Magneto-electric Composite

Multiferroic materials combine two or more ferroic characteristics and can exhibit an interaction between electric and magnetic fields. Since most magneto-electric (ME) single-phase materials show a technical irrelevant interaction between electric polarization and magnetization, the design of two-phase composites, consisting of a ferroelectric matrix with magnetostrictive inclusions, becomes important. As a result of the product properties within the composite, a strain-induced polarization/electrically activated magnetization is observed. In order to determine the effective properties a two-scale finite element (FE^2) homogenization approach is performed. Furthermore, the nonlinear properties of the ferroelectric phase are approximated with an appropriate material model.

Joerg Schroeder
Uni Duisburg Essen
Institut f. Mechanik, Abteilung Bauwissenschaften
j.schroeder@uni-due.de

Matthias Labusch
UDE
matthias.labusch@uni-due.de

MS92

Finite Temperature Behavior of Crystalline Defects in the Thermodynamic Limit

I will present an analytical framework that allows one to rigorously study properties of defects, such as local observables or defect density, at the thermodynamic limit. I will then show how to use this framework to also study accuracy of coarse-graining of molecular models at finite temperature. Application to direct molecular modelling and the hot-quasicontinuum method will be presented.

Alexander Shapeev
Skolkovo Institute of Science and Technology
shapeev@gmail.com

Mitchell Luskin
School of Mathematics
University of Minnesota
luskin@umn.edu

MS93

Using Causality in Microelectronics Modeling

Design of microelectronic systems requires systematic simulations of suitable causal models that capture relevant electromagnetic phenomena that affect signal and power quality. These models are obtained from discrete bandlimited frequency responses using macromodeling techniques. Causality can be expressed using Hilbert transform. Having bandlimited data causes significant boundary artifacts. We use Fourier continuations to completely remove boundary artifacts and enforce causality. The approach is extended to time delay estimation and study of accurate conversion from single-ended to mixed-mode S parameters.

Lyudmyla Barannyk
University of Idaho
Department of Mathematics
barannyk@uidaho.edu

MS93

Numerical Verification of the Bond-Based Peridynamic Softening Model Against Classical Theory

We focus on the bond-based Peridynamic Softening [1] model with respect to small deformations. In this model the material parameters are obtained by the Γ-convergence and are independent of the size of the interaction zone. Thus, the length scale of the nonlocal interaction is not a discretization parameter and instead describes a length scale associated with the process zone of the material. We present how to connect the model parameters with energy equivalence to common material parameters from classical theory. To verify the numerical discretization (EMU-PD) and the implementation we demonstrate that the Softening model reproduces the Young's modulus and the Poisson's ratio with respect to the classical theory. Another aspect is that the applied discretization conserves the Peridynamic model energy, obtained from the classical theory, independent of the size of the non-local interaction zone.

[1] R. Lipton, Dynamic Brittle Fracture as a Small Horizon Limit of Peridynamics, Journal of Elasticity, 2014, Volume 117, Issue 1, pp 21-50.

Patrick Diehl
Universität Bonn
Institut für Numerische Simulation
diehl@ins.uni-bonn.de

Robert P. Lipton
Department of Mathematics
Louisiana State University
lipton@math.lsu.edu

Marc Alexander Schweitzer
INS / Meshfree Multiscale Methods
University of Bonn / Fraunhofer SCAI
schweitzer@ins.uni-bonn.de

MS93

Nonlocal Higher Order Operators and Convergence

to Their Classical Counterparts

In this talk we will present some results on a nonlocal operator introduced as a natural generalization to the biharmonic operator that appears in plate theory. This operator is built in the nonlocal calculus framework and is connected with the recent theory of peridynamics. For the steady state equation coupled with different boundary conditions we show existence and uniqueness of solutions, as well as regularity of solutions. The boundary conditions considered are nonlocal counterparts of the classical clamped and hinged boundary conditions. For each system we show convergence of the nonlocal solutions to their local equivalents using compactness arguments developed by Brezis, Bourgain, Mironescu.

Petronela Radu
University of Nebraska-Lincoln
Department of Mathematics
pradu@math.unl.edu

Daniel Toundykov
Department of Mathematics
University of Nebraska-Lincoln
dtoundykov@unl.edu

Jeremy Trageser
George Washington University
jtrageser@email.gwu.edu

MS94

The Mesh-Particle Coupling Tool MaMiCo for Multi-Resolution Fluid Dynamics: Flexibility, Parallelism, and Multi-Instance Sampling

Hybrid mesh-particle simulation methods in fluid dynamics allow to resolve some parts of the computational domain using particles, and other parts of the domain by means of a (potentially) coarse-grained mesh-based solver. We have developed the macro-micro-coupling tool MaMiCo to provide a flexible, modular and parallel piece of software to couple mesh-based flow solvers and particle-based, e.g. molecular dynamics (MD), simulations. We discuss functionality and performance of the tool by coupling four molecular dynamics codes (SimpleMD, ls1 mardyn ESPResSo, LAMMPS) and the spatially adaptive Lattice Boltzmann (LB) solver waLBerla. We provide details on the MaMiCo interface implementations and validate them by considering a state-based molecular-continuum simulation of channel flow. We further show strong scaling results for different simulation scenarios. Coupling a single mesh-based solver instance to several identical particle-based solver instances allows for averaging over totally independent particle samples as well as for embarrassing parallelism on the side of the computationally very intensive particle-based solvers. We demonstrate how to set up a respective simulation using MaMiCo at the example of LB-DPD coupling.

Philipp Neumann
Technische Universität München, Germany
Scientific Computing in Computer Science
neumanph@in.tum.de

X Bian
Brown University
xin_bian@brown.edu

MS94

Adaptive Dual-Resolution Simulation Methods for Soft Matter: Where From, Where To?

In recent years there has been a considerable development of computational strategies to simulate soft matter concurrently employing two representations of the same system having different degrees of detail. These methods, aiming at reducing the computational cost of simulations, proved also to be valuable tools to investigate soft matter systems. In this talk I will provide an overview of dual-resolution simulation strategies, and discuss relevant applications and future developments.

Raffaello Potestio
Max Planck Institute for Polymer Research
potestio@mpip-mainz.mpg.de

MS94

Synchronized Molecular-Dynamics Simulation via Global Heat and Momentum Transports

The Synchronized Molecular-Dynamics simulation which was recently proposed by authors [Phys. Rev. X **4**, 041011 (2014)] is applied to the thermal polymer lubrication between parallel plates. In the SMD method, many MD cells are assigned to the local fluid elements to calculate the local molecular states, but they are synchronized at certain time intervals to satisfy the global heat and momentum transports over the whole domain. The rheological behaviors coupling with the viscous heating and conformational change are demonstrated.

Shugo Yasuda
University of Hyogo
yasuda@sim.u-hyogo.ac.jp

Ryoichi Yamamoto
University of Kyoto
ryoichi@cheme.kyoto-u.ac.jp

MS95

Exploration of Multi Phase, Multi Component Thermodynamic Spaces As Solutions to Constraint Satisfaction Problems

When it comes to the exploration of multi-dimensional phase stability spaces there is a large class of problems that need to be defined in terms of the satisfaction of a set of non-linear constraints. In this work we present a novel formulation for the exploration of multi-compoment systems as a constraint satisfaction problem. We present some preliminary algorithms aimed at solving the problem and provide some examples of their application.

Ray Arroyave, Sean Gibbons, Edgar Galvan, Richard Malak
Texas A&M University
rarroyave@tamu.edu, sean.l.gibbons@gmail.com, e.galvan3205@gmail.com, rmalak@tamu.edu

MS95

Towards Automation of Phase Diagram Calculation

Some challenges in calculation of phase diagrams stem from

the lack of a priori knowledge and data uncertainty, while others are related to running numerical optimization in the presence multiple local minima. These factors combined make thermodynamic assessments tedious and often highly unreliable. Driven by the desire to mitigate these challenges, we propose a unified framework capable of handling the task with minimal user input. The new methodology is implemented in AMPL and the results are compared and contrasted with existing literature.

Igor Griva, Maria Emelianenko, Jeff Snider
George Mason University
igriva@gmu.edu, memelian@gmu.edu, jeff@snider.com

MS95

The CALPHAD Gibbs Energy Minimization Challenge

Gibbs energy minimization using Lagrange functions strongly depends on start values and is susceptible to finding a local minimum rather than global minimum (true equilibrium). Although there are different approaches to address this problem, not all of them are practical for calculating materials containing six or more components. Gridpoint methods that calculate the Gibbs energy of all phases at many gridpoints find the global minimum but do not provide derivatives that simulation applications need.

Ursula Kattner
NIST
ursula.kattner@nist.gov

MS95

Use of Extended Gibbs Energy Algorithms for Constrained Phase Equilibria and New Kind of Phase Diagrams"

The Constrained Gibbs Free energy (CFE) technique provides a quantitative methodology for such chemical and phase changes which are affected by specific physical functions deciphered as thermodynamic work or which are restricted by non-equilibrium affinities. Based on computational multiphase thermodynamics, the method allows for a range of applications including construction of new kinds of phase diagrams for partial and paraequilibrium systems and for systems influenced by external fields or constrained by extent of chemical reactions.

Pertti S. Koukkari
VTT Process Chemistry, Finland
pertti.koukkari@vtt.fi

Risto Pajarre
VTT Process Chemistry, Finland
Senior Research Scientist
risto.pajarre@vtt.fi

MS96

Nonlinear Dynamics in Microscale Granular Crystals

Granular media support rich acoustic phenomena that stem from their complex microstructure and highly nonlinear particulate interactions. In this work, we study the contact-based dynamics of ordered and reduced dimensional microscale granular systems. Using laser ultrasonic techniques, we excite vibrations in monolayers of microspheres adhered to substrates, and observe a nonlinear dynamic response. This work opens the door for the study of microscale granular crystals and the design of new self-assembled passive wave tailoring devices.

Nicholas Boechler
University of Washington
Department of Mechanical Engineering
boechler@uw.edu

MS96

From Energy Cascades and Woodpile Chains to Disordered Media and Origami Lattices

In this talk, we will provide an overview of results in granular crystals, consisting of (monomer or dimer) beads interacting through Hertzian contacts. We will discuss highly localized traveling waves, as well as states in the form of (dark) discrete breathers and shock waves. In the last part of the talk, time-permitting, a number of recent aspects will be touched upon including: (a) formation of traveling waves with non-vanishing tails in elastic woodpile periodic structures; (b) super-diffusive transport in disordered granular chains; (c) applications of these lattices for the demonstration of switching and acoustic logic gates; (d) prototypical examples of extensions to two dimensions in hexagonal, as well as square arrays.

Panayotis Kevrekidis
University of Massachusetts
kevrekid@math.umass.edu

MS96

From Noisy Signals to Solitary Wave Trains

An extended time, noisy input perturbation at one end of a long granular chain ends up as a sequence of propagating solitary waves in the chain and eventually as a solitary wave train. Early work suggested that the peaks in the solitary wave train decay approximately exponentially. A precise form to describe the sequence of peaks remained elusive. Here we shall discuss how the properties of the input and material parameters relate to strains associated with the solitary wave train. The system could provide a way to convert noisy energy sources to useful ones.

Sourish Chakravarty
Dept of Mechanical and Aerospace Engineering
State University of New York at Buffalo
sourish.chakravarty@gmail.com

Surajit Sen
SUNY Buffalo
sen@buffalo.edu

MS96

Nonlinear Wave Dynamics in Origami-based Mechanical Metamaterials

We investigate unique nonlinear wave dynamics in origami-based mechanical metamaterials composed of volumetric 3D origami unit cells, such as Tachi Miura Polyhedron and Kresling origami. By using numerical simulations, we show that these mechanical systems can support rich phenomena of nonlinear wave dynamics, such as rarefaction wave formation and nonlinear wave mixing effects. We will also introduce ongoing efforts on experimental verifications of such nonlinear wave dynamics using various prototypes of

origami-based mechanical metamaterials.

Hiromi Yasuda
Department of Aeronautics and Astronautics
University of Washington
hiromy@uw.edu

Christopher Chong
Bowdoin College
cchong@bowdoin.edu

Panayotis Kevrekidis
University of Massachusetts
kevrekid@math.umass.edu

Jinkyu Yang
University of Washington
jkyang@gmail.com

MS97

Spectral Theory with Out Ellipticity: Bloch Waves and Separation of Frequency Spectra

Analytic representation formulas and power series are developed describing the band structure inside periodic photonic and acoustic crystals made from high contrast inclusions. Central to this approach is the identification of a resonance spectrum for quasi-periodic source free modes. This is used to determine bounds on the contrast that control the convergence radius of the series. These conditions are shown to be sufficient for the separation of spectral branches of the dispersion relation.

Robert P. Lipton, Robert Viator Jr.
Department of Mathematics
Louisiana State University
lipton@math.lsu.edu, rviato2@lsu.edu

MS97

Gap Solitons in Almost Periodic One-Dimensional Structures

We discuss the existence of gap solitons in certain model of almost periodic one dimensional photonic crystals. Mathematically the problem reduces to the existence of a nontrivial finite energy solution to almost periodic nonlinear Schrödinger equations in the case when 0 belongs to a finite spectral gap of the linear part.

Alexander Pankov
Department of Mathematics
Morgan State University, Baltimore
alexapankov@gmail.com

MS97

Boundary Value Problems for the Anistropic Maxwell System in Lipschitz Domains

Session code: L; Oral; Yes, you can transfer to poster. Boundary value problems for the time-dependent, anisotropic Maxwell system are analyzed in a bounded, Lipschitz domain in $\mathbb{R}^3$. The permittivity ε and the permeability μ are parameters which determine the propagation of radiation in a material, and here are assumed to be 3×3 matrices depending on position. Each element $\varepsilon_{ij}(x)$ and $\mu_{ij}(x)$ is assumed to be only bounded and measurable; no differentiability of these parameters is assumed.

Eric Stachura
Temple University
eric.stachura@temple.edu

MS97

Efficient Solvers for Electromagnetic Wave Propagation Problems in Complex Geometries

Abstract not available

Catalin Turc
Department of Mathematical Sciences
New Jersey Institute of Technology
catalin.c.turc@njit.edu

MS98

On Weak Anchoring for a Two-Dimensional Nematic Liquid Crystal

We study the weak anchoring condition for nematic liquid crystals in the context of the Landau-De Gennes model. We restrict our attention to two dimensional samples and to nematic director fields lying in the plane, for which the Landau-De Gennes energy reduces to the Ginzburg–Landau functional, and the weak anchoring condition is realized via a penalized boundary term in the energy. We study the singular limit as the length scale parameter $\epsilon \to 0$, assuming the weak anchoring parameter $\lambda = \lambda(\epsilon) \to \infty$ at a prescribed rate. We also consider a specific example of a bulk nematic liquid crystal with an included oil droplet and derive a precise description of the defect locations for this situation, for $\lambda(\epsilon) = K\epsilon^{-\alpha}$ with $\alpha \in (0, 1]$. We show that defects lie on the weak anchoring boundary for $\alpha \in (0, \frac{1}{2})$, or for $\alpha = \frac{1}{2}$ and K small, but they occur inside the bulk domain Ω for $\alpha > \frac{1}{2}$ or $\alpha = \frac{1}{2}$ with K large.

Stan Alama, Lia Bronsard
McMaster University
Department of Mathematics and Statistics
alama@mcmaster.ca, bronsard@mcmaster.ca

Bernardo Galvao-Sousa
Department of Mathematics
University of Toronto
beni@math.toronto.edu

MS98

Geometrically Nonlinear Models for Nematic Elastomers

We will discuss recent models for nematic elastomers by Barchiesi-DeSimone and by Calderer-Garavito-Yan, which involve simultaneously an elastic energy defined in the reference configuration and an energy that penalizes spatial variations of the nematic orientation in the deformed configuration. A local invertibility property for orientation-preserving Sobolev maps is used in order to establish the existence of minima. We present a refinement of the theories in which the hypotheses on the coercivity of the energy functions are slightly weakened. This is made possible by the results on the regularity of the inverses of Sobolev maps obtained by Henao and Mora-Corral in the analysis of cavitation and fracture in nonlinear elasticity.

Marco Barchiesi

Università degli Studi di Napoli Federico II
marco.barchiesi@unina.it

Duvan Henao
Pontificia Universidad Catolica de Chile
dhenao@mat.puc.cl

Carlos Mora-Corral
Department of Mathematics
Univerisity Autonoma
carlos.mora@uam.es

MS98

Limits of minimizers of a Landau-de Gennes functional

In this talk we discuss some properties of limits of minimizers of a Landau-de Gennes energy functional. These limits are singular harmonic maps, and we give a crude description of the singularity.

Alberto Montero
Departamento de Matematica
Pontificia Universidad Católica de Chile
amontero@mat.puc.cl

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

MS98

Point Defects in the Landau-de Gennes Model: Qualitative Features and Stability

We will present recent work on the point defects in the Q-tensor framework, both in 2d and 3d, focusing on qualitative features and energetic stability. We will also explore the relationships with the underlying Oseen-Frank theory. This is based on several works done in collaborations with Giovanni di Fratta, Radu Ignat,Georgy Kitavtsev, Luc Nguyen, Jonathan Robbins and Valeriy Slastikov.

Arghir Zarnescu
University of Sussex,
a.zarnescu@sussex.ac.uk

MS99

Quantized Vortex Dynamics and Interaction in Superfluidity and Superconductivity on Bounded Domains

Quantized vortices have been experimentally observed in type-II superconductors, superfluids, nonlinear optics, etc. In this talk, I will review different mathematical equations for modeling quantized vortices in superfluidity and superconductivity on bounded domains, including the nonlinear Schrodinger/Gross-Pitaevskii equation, Ginzburg-Landau equation, nonlinear wave equation, etc. Asymptotic approximations on single quantized vortex state and the reduced dynamic laws for quantized vortex interaction are reviewed and solved approximately in several cases. Efficient and accurate numerical methods will be presented for computing quantized vortex lattices and ther dynamics. Direct numerical simulation results from different PDE models are reported for quantized vortex dynamics on bounded domains and they are compared with those from the reduced dynamics laws. Some open problems and emerging applications will be discussed. This is a joint work with Qinglin Tang.

Weizhu Bao
National University of Singapore
Department of Mathematics
matbaowz@nus.edu.sg

MS99

Multiscale Model for Interlayer Dislocations in Bilayer Graphene

We present a multiscale model to describe the interlayer dislocations in bilayer materials. The model incorporates both the elasticity of each layer and the first-principle calculation informed interaction between two layers. We apply this approach to determine the structure and energetics of interlayer dislocations and twist grain boundaries in bilayer graphene. Our multiscale model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

Shuyang Dai
University of Pennsylvania
shuyangd@seas.upenn.edu

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

David J. Srolovitz
University of Pennsylvania
srol@seas.upenn.edu

MS99

Blended Atomistic-to-Continuum Hybrid Methods for Modeling Crystalline Materials

The development of consistent and stable atomistic-to-continuum coupling models for multi-dimensional crystalline solids remains a challenge. In this talk, we consider force-based atomistic-to-continuum coupling methods of blending type: the force-based quasicontinuum methods, with a comprehensive error analysis that is valid in two and three dimensions, for simple crystals, and in the presence of lattice defects (point defects and dislocations). Recently, we extend our analysis to multi-lattices crystals, for example, graphene type structures. Based on a precise choice of blending mechanism, the error estimates are considered in terms of degrees of freedom. The numerical experiments for simple crystals confirm the theoretical predictions.

Xingjie Li
University of North Carolina at Charlotte
xli47@uncc.edu

Brian Van Koten
The University of Chicago
vankoten@galton.uchicago.edu

Mitchell Luskin, Derek Olson
School of Mathematics
University of Minnesota
luskin@math.umn.edu, olso4056@umn.edu

Christoph Ortner
University of Warwick

christophortner0@gmail.com

Alexander Shapeev
Skolkovo Institute of Science and Technology
shapeev@gmail.com

MS99

Mathematical Modeling and Analysis of Plasmonic Nanoparticles

We propose a framework for mathematical modeling and analysis of plasmonic nanoparticles. The main purpose is to analyze the shift and broadening of the plasmon resonance with changes in size and shape of the nanoparticle. Both Helmholtz and Maxwell models are considered.

Hai Zhang
Hong Kong University of Science and Technology
haizhang@ust.hk

MS100

Producing Nanodot Arrays with Improved Hexagonal Order by Patterning Surfaces Before Ion Sputtering

When the surface of a flat binary material is bombarded with a broad, normally-incident ion beam, disordered hexagonal arrays of nanodots can form. Using numerical simulations, we investigate the influence of initial conditions on the hexagonal order achieved at long times. The initial conditions studied are hexagonal and sinusoidal templates, straight scratches and flat surfaces. Our simulations indicate that, under certain conditions, pre-patterning the surface can lead to significant improvements in the hexagonal order. The order is characterized using a topological data analysis technique called persistent homology.

Daniel A. Pearson, Richard Bradley
Colorado State University
Department of Physics
dan.pearson@colostate.edu, mark.bradley@colostate.edu

Francis Motta
Duke University
Department of Mathematics
francis.c.motta@gmail.com

Patrick Shipman
Department of Mathematics
Colorado State University
shipman@math.colostate.edu

MS100

Asymmetric Shape Transitions of Epitaxial Quantum Dots from Pyramid to Multifaceted Dome

We construct a two-dimensional continuum model to describe the energetics of shape transitions in fully-faceted epitaxial islands. The energetics of the shape transitions are determined by numerically calculating the facet lengths that minimize the energy of a given island type for prescribed island volume. By comparing the energy of different island types and analyzing the energy, we determine the bifurcation diagram of equilibrium solutions and their stability, as well as the lowest-barrier transition pathway.

Chaozhen Wei
State University of New York at Buffalo
cwei4@buffalo.edu

Brian J. Spencer
University at Buffalo
Department of Mathematics
spencerb@buffalo.edu

MS101

Active Control for the Helmholtz Equation by Almost Non-Radiating Solutions

We consider controlling the field generated by a solution to the Helmholtz equation in $\mathbb{R}^3$. We investigate how one can choose a mixed layer potential density on an antenna (or array of antennas) so that the induced field cancels a given incident field on some nearby control region, while simultaneously ensuring that far away it is suitably small. Numerical results will be presented, which extend previous work in the case of $\mathbb{R}^2$.

Mark Hubenthal
Institute for Mathematics and its Applications
hubenthal@ima.umn.edu

Daniel Onofrei
University of Houston
onofrei@math.uh.edu

MS101

Model Order Reduction in Inverse Problem for Maxwell's Equations

The work develops a model order reduction method for a numerical solution of multi-frequency electromagnetic forward and inverse problems using a rational interpolation of the transfer function in the complex plane. As the operator has a non-empty nullspace the problem is ill-posed. We regularize it by decomposing the equation into the part in the nullspace and the part orthogonal to it and by forcing the approximation to be exact on the nullspace.

Michal A. Kordy
Department of Mathematics, University of Utah
Energy & Geoscience Institute, University of Utah
kordy@math.utah.edu

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

Phil Wannamaker
University of Utah
wannamaker@egi.utah.edu

MS101

Nonlinear Imaging with Waves via Model Order Reduction

We introduce a novel nonlinear method for imaging with waves based on model order reduction. The reduced order model (ROM) is an orthogonal projection of the wave equation propagator on the subspace of time domain snapshots of solutions of the wave equation. It can be computed entirely from the knowledge of the time domain data measured on an array of transducers. The image is extracted from a backprojection of the ROM using the subspace basis for a known smooth kinematic velocity model. ROM

construction is based on an implicit orthogonalization of solution snapshots with a Gram-Schmidt procedure that respects the causality of the wave equation. This nonlinear procedure differentiates our approach from conventional linear imaging methods (Kirchhoff, reverse time migration). It allows for automatic removal of multiple reflection artifacts. It also doubles the resolution in range compared to conventional time reversal.

Alexander V. Mamonov
University of Houston
mamonov@math.uh.edu

Vladimir L. Druskin
Schlumberger-Doll Research
druskin1@slb.com

Andrew E. Thaler
Institute for Mathematics and its Applications
andythaler05@gmail.com

Mikhail Zaslavsky
Schlumberger-Doll Research
mzaslavsky@slb.com

MS101

On the Discreteness of the Interior Transmission Eigenvalues

In this talk, I will review know results on the discreteness of transmissions eigenvalues and discuss new ones.

Hoai-Minh Nguyen
École Polytechnique Fédérale de Lausanne
hoai-minh.nguyen@epfl.ch

Quoc Hung Nguyen
EPFL
quoc-hung.nguyen@epfl.ch

MS102

Practices of Coarse-Graining Based on the Mori-Zwanzig Formalism

We constructed coarse-grained force field directly from a multiscale dynamics via the Mori-Zwanzig (MZ) formulation. The MZ formalism for coarse-graining a complex dynamical system typically introduces memory effects. Using the Markovian assumption of Delta-correlated random forces, a dissipative particle dynamics (DPD) model can be obtained. Otherwise, a memory kernel of non-conservative force leads to a non-Markovian DPD (NM-DPD). Quantitative comparisons between the CG models with Markovian and non-Markovian approximations will be presented and discussed.

Zhen Li
Brown University
Brown University
Zhen_Li@brown.edu

Xin Bian
Brown University
Xin_Bian@brown.edu

Xiantao Li
Department of Mathematics
Pennsylvania State University
xli@math.psu.edu

George Em Karniadakis
Brown University
george_karniadakis@brown.edu

MS102

Radial Basis Function Methods for Meshfree Transport on the Sphere and Other Surfaces

We present novel Radial Basis Function (RBF) methods for meshfree transport on the sphere and other surfaces. As is typical of RBF methods, our methods work purely with Cartesian nodes. However, while current RBF methods require stabilization via carefully-tuned hyperviscosity operators, our new methods are intrinsically stable. We present results showing high orders of spatial convergence on the sphere, and demonstrate the ability of our methods to handle transport on arbitrary surfaces.

Varun Shankar
Department of Mathematics
University of Utah
vshankar@math.utah.edu

Grady B. Wright
Department of Mathematics
Boise State University, Boise ID
gradywright@boisestate.edu

MS102

Fundamental Studies of Dynamic Fracture with Multiscale Peridynamics

Peridynamics is an extension of the classical theory of solid mechanics that is oriented toward problems with evolving discontinuities, especially growing cracks. This talk will report on application of a concurrent hierarchical multiscale peridynamic code to the simulation of instabilities in dynamic fracture. These instabilities can produce features such as the mirror-mist-hackle transition. The talk will also cover a coarse-graining technique within peridynamics that adapts material models to changes in length scale.

Stewart Silling
Sandia National Laboratories
sasilli@sandia.gov

MS102

A Monolithic Compatible Meshless Discretization for Simulating Electrophoretic Suspensions

We present a new meshless discretization that generalizes staggered primal/dual discretizations to a graph to obtain a stable, high-order, compact approximation of the Stokes and Poisson-Boltzmann equations for arbitrary curvilinear geometry. We use these discretizations to study electrophoresis of colloidal suspensions, where the solution of a single monolithic system provides all details of the colloid dynamics, the electric field, and the flow variables.

Nathaniel Trask
Brown University
Division of Applied Mathematics

nathaniel_trask@brown.edu

MS103

Seamless Coupling of Nonlocal and Local Models

Nonlocal models are gaining popularity in multiscale modeling. To reduce the added computational cost due to nonlocal interactions, there are advantages to employ local models wherever they provide valid descriptions of the physical processes. To implement such concurrently coupled local and nonlocal models, it is important to construct suitable interfaces between nonlocal models (given by integral equations) and local ones (represented by PDEs). In this talk, we first present some new analytical results that help us formulating some well-defined coupled models. We then demonstrate how the recently developed framework of asymptotically compatible schemes can offer robust simulations of such models.

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

Yunzhe Tao
Department of Applied Physics and Applied Mathematics
Columbia University
y.tao@columbia.edu

Xiaochuan Tian
Columbia University
Department of Applied Physics and Applied Mathematics
xt2156@columbia.edu

MS103

Second Order Gamma-Convergence for the Modica Mortola Functional

The asymptotic behavior of an anisotropic Cahn-Hilliard functional with prescribed mass and Dirichlet boundary condition is studied when the parameter that determines the width of the transition layers tends to zero. The first order term in the asymptotic development by Gamma-convergence is well-known, and is related to a suitable anisotropic perimeter of the interface. Here it is shown that, depending on symmetry and growth hypotheses on the double well potential, the second order term in the Gamma-convergence expansion is zero. Slow motion is addressed, and related estimates of the rate of convergence of solutions of the associated Allen-Cahn equation to the minimum value are discussed.

Irene Fonseca
Carnegie Mellon University
Center for Nonlinear Analysis
fonseca@andrew.cmu.edu

MS103

Variational Convergence for the Analysis of Boundary Layers in Dislocation Pileups

It is a major challenge to connect a microscopic description of dislocation movement on one hand with models of macroscopic plastic behaviour on the other hand. At this stage we are not able to do this; there is a major gap between the models at these different spatial and temporal scales. In this talk I will report on a much more modest result. Dislocations 'pile up' at boundaries of the grains, through which they can not easily pass. These pileups give rise to a net force on the grain boundary, which can have macroscopic consequences. In this talk we study these pileups, and give a description at two levels, corresponding to a 'bulk' behaviour and a boundary-layer behaviour.

Patrick Van Meurs
Kanazawa University
Japan
pmeurs@staff.kanazawa-u.ac.jp

Adriana Garroni
Universita' di Roma
garroni@mat.uniroma1.it

Mark Peletier
Technische Universiteit Eindhoven
m.a.peletier@tue.nl

Lucia Scardia
University of Bath
Dept of Mathematical Sciences
l.scardia@bath.ac.uk

MS103

A Continuum Model for Dislocation Dynamics in Three Dimensions Using the Dislocation Density Potential Functions

We present a dislocation-based three-dimensional continuum model, in which the dislocation substructures are represented by two families of dislocation density potential functions (DDPFs), denoted by ϕ and ψ. The slip planes of dislocations are thus characterized by the contour surfaces of ψ, while the dislocation curves on each slip plane are identified by the contour curves of ϕ on that plane. The geometries and the density distribution of the dislocation ensembles are simply expressed in terms of the spatial derivatives of the DDPFs. The dynamics equations based on DDPFs are derived from the discrete dislocation dynamics, and include a constitutive stress rule describing how the stress field associated with dislocation networks is determined, and a plastic flow rule governing the dynamics of the dislocation ensemble.

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

Yichao Zhu
Department of Mathematics
The Hong Kong University of Science and Technology
mayczhu@ust.hk

MS104

Geometry of Thin Nematic Elastomer Sheets

Session Code AP, ORAL Thin nematic elastomer sheets attain 3D configurations that depend on the nematic director field upon heating. In this talk we describe the intrinsic geometry that is induced on such a sheet by any smooth director field. We investigate the reverse problem of constructing a director field that induces a specified 2D geometry, and provide analytical solutions for certain classes of desired geometries. We demonstrate how arbitrary 2D geometries can be designed using approximate numerical methods.

Hillel Aharoni

The Racah Institute of Physics
The Hebrew University of Jerusalem
haharoni@sas.upenn.edu

Eran Sharon
Hebrew University of Jerusalem
erans@mail.huji.ac.il

Raz Kupferman
Hebrew University
Israel
raz@math.huji.ac.il

MS104

Nonclassical Analysis of the Nonlinear Kompaneets Equation

The nonlinear Kompaneets (NLK) equation describes the spectra of photons interacting with a rarefied electron gas. We exhibit five previously unknown classes of explicit time-dependent solutions (each class depending on initial conditions with two parameters) of the NLK equation. It is shown that these solutions cannot be found as invariant solutions using the classical Lie method (solutions obtained by Ibragimov (2010)) but are found using the nonclassical method. Interestingly, each of these new solutions can be expressed in terms of elementary functions. Three of these solution classes exhibit quiescent behaviour and the other two solution classes exhibit blow-up behaviour in finite time. As a consequence, it is shown that corresponding nontrivial stationary solutions are all unstable. In the nonclassical method, one seeks "symmetries" that are transformations leaving invariant a solution submanifold of a given PDE system, i.e., "symmetries" that are transformations mapping some solutions of a given PDE system into solutions of the same system but map other solutions of the given PDE system map to solutions of a different PDE system, and then seeks corresponding solutions that are invariant. Consequently, all solutions obtainable by Lie's classical method can be obtained by the nonclassical method. This is joint work with Zhengzheng Yang and Shou-fu Tian. For details, see our paper with the same title in J. Eng. Math 84: 87-97 (2014)

George Bluman
Dept. of Mathematics
Univ. of British Columbia
bluman@math.ubc.ca

MS104

Nonlinear Elastodynamic Models of Wave Propagation and Conservation Laws for Fiber-Reinforced Materials

Constitutive models of incompressible fiber-reinforced hyperelastic and viscoelastic materials are used to derive nonlinear wave equations compatible with the incompressibility assumption. Equivalence transformations are employed to simplify the equations and to reduce the number of parameters. Local conservation laws and global conserved quantities are systematically computed in various settings. This work is joint with Jean-Francois Ganghoffer (U. Lorraine).

Alexei F. Cheviakov
Department of Mathematics and Statistics
University of Saskatchewan
cheviakov@math.usask.ca

MS104

Computation of the Effective Nonlinear Mechanical Response of Lattice Materials Considering Internal Scale Effects

The asymptotic homogenisation technique is developed in the framework of geometrical nonlinearities to derive the large strains effective elastic response of network materials viewed as repetitive beam networks. This systematic methodology allows the prediction of the overall mechanical properties of these structures in the nonlinear regime, reflecting the influence of the geometrical and mechanical micro-parameters of the network. Internal scale effects are captured by consideration of a micropolar effective continuum model. Applications to the computation of the large strains response of auxetic planar and 3D lattices exemplify the powerfulness of the proposed method.

Jean-François Ganghoffer
LEMTA, INPL Nancy
jean-francois.Ganghoffer@univ-lorraine.fr

Jean-François Ganghoffer
LEMTA, Université de Lorraine
jean-francois.Ganghoffer@univ-lorraine.fr

MS105

Global Energy Minimization of Multi-Component Phases with Internal Degrees of Freedom

Miscibility gap detection is a crucial feature in thermodynamic calculation software to accurately calculate the energy of phases containing regions of compositional instability and is commonly handled through global minimization of the Gibbs energy function. In multi-component systems the topology of the energy surfaces can become quite complex, since the high-dimensional tangent hyperplanes which define equilibrium can interact with the energy surface in more complicated ways. Here methods for solving the multi-component case with multiple sublattices will be discussed, along with an approach using quasi-random sequences for ensuring uniform sampling of a phase's internal degrees of freedom.

Richard Otis
Pennsylvania State University
rao140@psu.edu

MS105

Numerical Challenges in Computing Thermodynamic Equilibria in Large Complex Systems and Upon Integration in Multi-Physics Codes

Computational thermodynamics plays an integral role in facilitating engineering design of a wide array of materials and processes. Recent trends are focused towards larger and more sophisticated representations of complex systems and the integration of thermodynamics calculations into multi-physics codes in order to enhance their predictive capabilities. The increasing computational complexity of thermodynamics models amplifies existing and introduces new numerical and algorithmic challenges. For instance, the ability to reliably ensure that a global minimum of the integral Gibbs energy function has been reached becomes increasingly difficult and computationally expensive for large systems due to the combinatorial nature and

multimodality of the problem. These concerns are augmented when thermodynamic computations are integrated in multi-physics codes, which place strict demands on their reliability and performance. Recent advancements in algorithm development for computational thermodynamics and application of global optimization methods will be discussed. Irradiated nuclear fuel, with its large number of fission products and phases, will be used as a vehicle to identify these challenges and demonstrate solutions.

Markus Piro
Canadian Nuclear Laboratories
markus.piro@cnl.ca

Srdjan Simunovic
Oak Ridge National Laboratory
simunovics@yahoo.com

MS106

A Molecular Dynamics Study on the Mechanics of the Lipid Bilayer Membrane Containing an Integrin Protein under Shock Loading.

Molecular dynamics simulations were carried out to study the effects of shockwaves on a lipid bilayer model with integrin embedded. The shockwave effect on the mechanical stability and structure of the lipid bilayer has been tested and analyzed. Along with this, the forces experienced during shockwaves by integrin, a protein involved in cell-matrix adhesions has been measured. The results helps elucidate the passive and active response of cell membranes and cells to shock load.

Ralph Kfoury, Hongyan Yuan
University of Rhode Island
ralph_kfoury@my.uri.edu, hongyan_yuan@uri.edu

MS106

Simulations of Particle Structuring Driven by Electric Fields

Recent experiments show intriguing surface patterns when a uniform electric field is applied to a droplet covered with colloidal particles. Depending on the particle properties and the field intensity, particles organize into an equatorial belt, pole-to-pole chains, or dynamic vortices. Here we present 3D simulations of the collective particle dynamics, which account for the electrohydrodynamicsand dielectrophoresis of particles. Results are presented for various physical parameters and comparison to experiment is done.

Michael Miksis
Department of Engineering Science and Applied Mathematics
Northwestern University
miksis@northwestern.edu

Yi Hu
Northwestern University
yihu2012@u.northwestern.edu

Petia Vlahovska
Brown University
petia_vlahovska@brown.edu

MS106

Dynamics and Thermal Fluctuations of Particles On/Near an Interface

Abstract not available

Paul Salipante
National Institute of Standards and Technology
paul.salipante@gmail.com

MS106

Mechanics of Cell Interaction with Two-Dimensional Nanomaterials

I will report our recent studies on the interaction between the cell membrane and 2D nanomaterials such as graphene nanosheets. Our theoretical analysis suggests that there are two fundamental modes of interaction between the cell membrane and 2D nanomaterials: near-perpendicular membrane penetration and parallel membrane attachment. I will discuss the underlying mechanisms and effects of the size and bending stiffness of nanomaterials on the interaction modes.

Xin Yi
School of Engineering, Brown University
xin_yi@brown.edu

MS107

Quantum Optics in Random Media

We consider the propagation of two-photon light in a random medium. We show that the Wigner transform of the two-photon amplitude obeys an equation that is analogous to the radiative transport equation for classical light. Using this result, we investigate the propagation of an entangled photon pair.

John Schotland
University of Michigan
schotland@umich.edu

MS107

Soliton Solutions of the Nonlinear Exciton-Polariton Equations

Abstract not available

Stephen P. Shipman
Department of Mathematics
Louisiana State University
shipman@math.lsu.edu

MS107

Existence and Stability Properties of Radial Bound States for Schrödinger-Poisson Equation with external Coulomb potential in Three Space Dimensions

We consider radial solutions to the Schrödinger-Poisson system in three dimensions with an external, smooth, potential with Coulomb-like decay. Such a system can be viewed as a model for the interaction of dark matter with a bright matter background in the non-relativistic limit. We find that there are infinitely many critical points of the Hamiltonian, subject to fixed mass, and that these bifurcate from solutions to the associated linear problem at zero mass. As a result, each branch has a different topological character defined by the number of zeros of the radial states. We construct numerical approximations to

these nonlinear states along the first several branches. The solution branches can be continued, numerically, to very large mass values, where they become asymptotic, under a rescaling, to those of the Schrödinger-Poisson problem with no external potential. Time dependent numerical simulations suggest that the ground state, as well as the excited states, are stable, subject to the radial symmetry restriction.

Jeremy L. Marzuola
Department of Mathematics
University of North Carolina, Chapel Hill
marzuola@math.unc.edu

Sarah Raynor
Wake Forest University
raynorsg@wfu.edu

Gideon Simpson
Department of Mathematics
Drexel University
simpson@math.drexel.edu

MS107

Weak Wave Turbulence in Systems with PT-Symmetry.

Session code: L; Oral; Yes, transfer to poster PT-symmetric systems is a hot research topic in the area of nonlinear optics. They can provide a new framework for a number of applications, e.g. in the transport-based devices such as particle separators or molecular switches. In this work I present some numerical results of weak wave turbulence in PT-symmetric systems.

Alexey Sukhinin
Southern Methodist University
asukhinin@smu.edu

MS108

Mathematical Descriptions of Point, Line and Surface Defects

The talk will consider different possibilities for describing point, line and surface defects as singularities having finite energy in director and line-field based models of liquid crystals.

John Ball
Oxford Centre for Nonlinear PDE Mathematical Institute
Oxford
ball@maths.ox.ac.uk

Stephen Bedford
University of Oxford
stephen.bedford@exeter.ox.ac.uk

MS108

A Topological Obstruction Related to Nematic Shells: Morse's Index Formula for VMO Vector Fields

We consider the following problem: Given a compact manifold N with boundary, which are the unit vector fields g, defined on the boundary of N, that can be extended to a $W^{1,p}$-unit vector field u, defined on N. This question is motivated by the analysis of variational models for a thin film of nematic liquid crystals spread on a surface. In the continuous setting, the answer depends on a topological obstruction, namely, Morse's index formula. Inspired by Brezis and Nirenberg's work on the topological degree, we extend Morse's formula to the class of VMO (Vanishing Mean Oscillation) functions. This yields a characterisation of the boundary data g that admit an extension with the required properties. This is joint work with Antonio Segatti and Marco Veneroni (Pavia, Italy).

Giacomo Canevari
Mathematical Institute, University of Oxford
Laboratoire Jacques Louis Lions, UPMC Paris 6
Giacomo.Canevari@maths.ox.ac.uk

MS108

Limiting Behaviors of Bent-Core Liquid Crystal Models

We will present preliminary analytical and numerical results related to an energy functional introduced in the physics literature to model bent-core molecule liquid crystals.

Tiziana Giorgi
Department of Mathematical Sciences
New Mexico State University
tgiorgi@math.nmsu.edu

Sookyung Joo
Old Dominion University
sjoo@odu.edu

Carlos J. Garcia-Cerver
UCSB
cgarcia@math.ucsb.edu

MS108

Dimension Reduction for the Landau-de Gennes Model of Nematic Films on Surfaces

I will present the dimension reduction procedure for the Landau-de Gennes model describing a nematic film deposited on a general surface. I will also discuss the structure of limiting-energy-minimizing configurations for some simple examples.

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

Peter Sternberg
Indiana University
Department of Mathematics
sternber@indiana.edu

Alberto Montero
Departamento de Matematica
Pontificia Universidad Católica de Chile
amontero@mat.puc.cl

MS109

Efficient Algorithms for Transition State Calculations

Transition states are fundamental to understanding the reaction dynamics qualitatively. To date various methods of first principle location of transition states have been devel-

oped. In the absence of the knowledge of the final structure, the minimal-mode following method climbs up to a transition state without calculating the Hessian matrix. In this talk, we introduce a locally optimal search direction finding algorithm and an iterative minimizing method for the translation which improve the rotational step by a factor and the translational step a quantitative scale. Numerical experiments demonstrate the efficiency of our proposed algorithms. This is joint work with Jing Leng, Zhi-Pan Liu, Cheng Shang and Xiang Zhou.

Weiguo Gao
Fudan University, China
wggao@fudan.edu.cn

MS109

Grain Boundary Roughening in Colloidal Crystals

We observed the grain-boundary roughening transition inside a bulk crystal for the first time using thermal-sensitive thin-film colloidal crystals. Single-particle dynamics inside the bulk can be directly visualized under the video microscopy. As the effective temperature decreases, the straight large-angle grain boundaries become rough with the strongest shape fluctuations at the roughening transition below the premelting point. The roughening transition exhibits both static and dynamical critical behaviors. We attribute the grain-boundary widening as the cause of the exotic decrease of the shape fluctuation and the mobility change of the grain boundary as approaching the premelting point. Small-angle grain boundaries exhibit different melting behaviors which prempty its roughening.

Yilong Han
Hong Kong University of Science and Technology
yilong@ust.hk

MS109

Grain Boundary Migration in Nanocrystalline Metals

Grain growth is usually modeled as mean curvature flow in an interconnected grain boundary network, where all grain boundaries are commonly assumed to have the same energies and mobilities. We perform molecular dynamics simulations of grain growth in nanocrystalline nickel, and observe a wide range of phenomena that occur during the coarsening of the polycrystalline microstructure. I will review and catalog many of these surprising phenomena and present a more holistic view of grain growth.

Spencer L. Thomas
University of Pennsylvania
Department of Materials Science and Engineering
slthomas61@gmail.com

David J. Srolovitz
University of Pennsylvania
srol@seas.upenn.edu

MS109

A Continuum Model for Dynamics of Dislocation Arrays and Applications to Low Angle Grain Boundaries

We present a continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries which may be nonplanar and nonequilibrium. We define a dislocation density potential function on the dislocation array surface or grain boundary to describe the orientation dependent continuous distribution of dislocations. The continuum formulation incorporates both the long-range dislocation interaction and the local dislocation line energy, and is derived from the discrete dislocation model. We also develop numerical methods to solve this continuum model.

Luchan Zhang, Yejun Gu
Hong Kong University of Science and Technology
lzhangas@connect.ust.hk, yguab@ust.hk

Xiaohong Zhu
Jinan University
maxhzhu@163.com

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

MS110

Wetting in Thin Solid Polycrystalline Films

We develop wetting criteria for three grains with bamboo structure constrained to lie within a prescribed triangular geometry, drawing conclusions based on existence and nonexistence of steady states, as well on relative energies. Results of numerical simulations are presented. Our results demonstrate the breakdown of the small slope approximation approach.

Vadim Derkach
Dept of Mathematics
Technion-Israel Institute of Technology
vadder@tx.technion.ac.il

John McCuan
Dept of Mathematics
Georgia Tech
mccuan@math.gatech.edu

Amy Novick-Cohen
Technion Israel Institute of Technology
amync@tx.technion.ac.il

MS110

Kinetics of the Triple Line in Solid-State Wetting

We analyze the kinetics of the triple-line of thin solid films during spreading or dewetting. We show that the departure from equilibrium at the triple line can be related to the kinetics at the micro or meso-scopic level. A continuum model is designed to describe triple in non-equilibrium situations. This model is related to non-equilibrium triple line kinetics via an asymptotic analysis. We discuss the influence of these findings on growth or dewetting dynamics.

Oliver Pierre-Louis
Université Claude Bernard Lyon 1
olivier.pierre-louis@univ-lyon1.fr

MS110

The Effect of Nanoindentation on Thermal Stabil-

ity and Dewetting of Thin Metal Films

Abstract not available

Eugen Rabkin
Technion Israel Institute of Technology
erabkin@techunix.technion.ac.il

MS110

Instabilities During Solid State Dewetting of Thin Films

The phenomenology of solid state dewetting as observed for single crystal films will be reviewed, with a focus on instabilities that develop at retracting edges. These include faceting and fingering instabilities, as well instabilities at corners of growing holes. Rayleigh-like break-up of stands will also be discussed. All of these phenomena are strongly affected by crystalline anisotropy in ways that are difficult to capture in models and simulations.

Carl V. Thompson
Massachusetts Institute of Technology
cthomp@mit.edu

MS111

Variational Principle for Probabilistic Measure in Theory of Materials with Random Microstructure

Materials with random microstructures can be adequately described only in probabilistic terms. One of the problems that arise is: how to find probabilistic characteristics of local fields (stresses, currents, etc.), if probability distributions of material characteristics are known? In the talk this problem is considered using the variational principle for probabilistic measure.

Victor Berdichevsky
Wayne State University
vberd@eng.wayne.edu

MS111

Transport Properties of a Periodic Array of Spherical Inclusions

We determine the effective tensor of a two-phase composite consisting of an arbitrary periodic lattice of identical spherical inclusions embedded in a homogeneous matrix whose physical properties are complex-valued. The approach is based on representation of the potential in terms of three-dimensional periodic harmonic functions. Analytical expression for the effective tensor is provided as a function of lattice sums and material parameters.

Yuri Godin
University of North Carolina at Charlotte
ygodin@uncc.edu

MS111

Disordered Hyperuniform Materials: Novel States of Amorphous Matter

Disordered hyperuniform many-body systems can be regarded to be new states of amorphous matter in that they behave more like crystals or quasicrystals in the manner in which they suppress large-scale density fluctuations, and yet are also like liquids and glasses because they are statistically isotropic structures with no Bragg peaks. I will describe the theory behind hyperuniformity and examples of disordered hyperuniform systems that arise in physics, mathematics and biology.

Salvatore Torquato
Chemistry and Princeton Center for Theoretical Science
Princeton University
torquato@electron.princeton.edu

MS111

Surface-Elasticity-Based Approach in Modeling Material Microstructure in Fracture Problems

A new model of fracture mechanics which takes into account interfacial effects due to a curvature-dependent surface tension will be considered. The theory will be presented through several examples: a curvilinear non-interface and interface crack, and contact problems for a rigid stamp indentation. It will be shown that the incorporation of surface effects on the crack boundary eliminates the power and oscillating singularities at the crack tips which are predicted by linear elastic fracture mechanics.

Anna Zemlyanova
Department of Mathematics
Kansas State University
azem@ksu.edu

MS112

Smoothed Particle Hydrodynamics: Consistence, Convergence and Transport-Velocity Formulation

The lack of consistence and convergence is often considered as a major drawback of smoothed particle hydrodynamics (SPH). We show that partition of unity is the condition under which the SPH approximation achieves both consistence and convergence, and show that this condition can be achieved by relaxing particle distribution. Based the analysis, we explain why our previously proposed transport-velocity formulation of SPH is able to achieve unprecedented accuracy and stability, and present the extension of the transport-velocity formulation to simulate solid dynamics problems with free material surfaces.

Xiangyu Hu
Technical University of Munich
xiangyu.hu@tum.de

MS112

Integral Approximations to Classical Diffusion and Smoothed Particle Hydrodynamics

Abstract not available

Richard B. Lehoucq
Sandia National Laboratories
rblehou@sandia.gov

MS112

Simulating Transport in Microfluidics and Porous Electrodes by Implicit Incompressible Smoothed Particle Hydrodynamics

This work focuses on the mathematical model and numerical scheme of implicit incompressible smoothed particle hydrodynamics, which can effectively capture multiphysics

including hydrodynamics, electrostatics, and advection-diffusion. The order of accuracy is significantly improved with the present implicit consistent numerical scheme. Specifically, we show simulation results on electrokinetic flows associated in applications of transport in microfluidics and porous electrodes.

Wenxiao Pan
Pacific Northwest National Laboratory
wenxiao.pan@pnnl.gov

Kyungjoo Kim
Sandia National Laboratories
kyukim@sandia.gov

Mauro Perego
CSRI Sandia National Laboratories
mperego@sandia.gov

MS112

Quantifying the Dynamics of Thermo-Responsive Polymers As Drug Delivery Vehicles

Using energy-conserving Dissipative Particle Dynamics, we uncovered the hidden dynamics of thermoresponsive drug carriers by simulating self-assembly processes triggered by spatial and temporal thermal variations. Two molecular movement modes dominate, namely ***flip*** and ***slip***, in thermoresponsive bilayer membranes during inversion. We identified a frequency regime where thermoresponsive vesicles survive thermal loading tests, and quantified the collapse probability for those didn't survive. We also observed that thermoresponsive carriers exhibit distinct hydrodynamics in flows of uneven temperature.

Yu-Hang Tang
Brown University
yuhang_tang@brown.edu

Zhen Li
Brown University
Brown University
Zhen_Li@brown.edu

Xuejin Li
Brown University
xuejin_li@brown.edu

Mingge Deng
Division of Applied Math, Brown University
mingge_deng@brown.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS113

Coarsening Dynamics for the Cahn-Hilliard Equation with Degenerate Mobility

We consider coarsening rates of the Cahn-Hilliard equation with a smooth double-well potential, and with phase-dependent diffusion mobilities. The latter is a feature of many materials systems and makes both theoretical analysis and accurate numerical simulations challenging. We first summarize our earlier theoretical predictions on the coarsening dynamics based on asymptotic analysis. Then we present numerical simulations that confirm the theoretical predictions. We demonstrate that the numerical solutions are consistent with the physical Gibbs–Thomson effect, even if the mobility is degenerate in one or both phases. For the two-sided degenerate mobility, we report computational results showing that the coarsening rate is on the order of $l \sim ct^{1/4}$, independent of the volume fraction of each phase. For the one-sided degenerate mobility, that is non-degenerate in the positive phase but degenerate in the negative phase, we illustrate that the coarsening rate depends on the volume fraction of the positive phase. For large positive volume fractions, the coarsening rate is on the order of $l \sim ct^{1/3}$ and for small positive volume fractions, the coarsening rate becomes $l \sim ct^{1/4}$.

Shibin Dai
Department of Mathematics
New Mexico State University
sdai@nmsu.edu

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

MS113

Propagation of Chaos for Many Particle Systems with Diffusion in Velocity

We consider large systems of particles interacting through rough but bounded interaction kernels. We are able to control the relative entropy between the N-particles distribution and the expected limit which solves the corresponding Vlasov system. This implies the Mean Field limit to the Vlasov system together with Propagation of Chaos through the strong convergence of all the marginals. The method works at the level of the Liouville equation and relies on precise combinatorics results.

Pierre-Emmanuel Jabin, Zhenfu Wang
University of Maryland
pjabin@cscamm.umd.edu, zwang@math.umd.edu

MS113

On the Existence and Regularity of Solutions to Euler's Equations for Hard Non-Spherical Particles

The construction and subsequent study of smoothness of solutions to Euler's equations for two hard spherical particles is straightforward and well understood. The analogous problem for *non-spherical particles* presents some surprising challenges. For instance, what is the maximum number of times two ellipsoidal particles can collide before complete separation? In this talk, we present some recent results (both analytical and numerical) on the existence and regularity of solutions to Euler's equations which have been obtained with Peter Palffy-Muhoray and Xiaoyu Zheng.

Mark Wilkinson
Courant Institute
mwilkins@cims.nyu.edu

Peter Palffy-Muhoray
Liquid Crystal Institute
Kent State University
mpalffy@cpip.kent.ed

Xiaoyu Zheng

Dept of Mathematics
Kent State University
zheng@math.kent.edu

MS113

1D Static Phase Field Crystals Coupled with Continuum Elasticity

The static phase field crystal (PFC) equation is a fourth order nonlinear elliptic equation that is obtained from a PFC energy as optimality condition. The local minimizers of that energy typically exhibit an oscillatory pattern consisting of several bumps arranged in a lattice (which may be interpreted as atoms in a crystalline material). If the period of the pattern deviates from the globally optimal period, e.g. due to boundary conditions, the PFC energy is increased. This increase can be viewed as a macroscopic elastic deformation energy. We present a numerical approach in 1D to parameterize the PFC function via this deformation and to couple a deformation-parameterized PFC to a non-parameterized PFC via an Arlequin-type approach.

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

Benedikt Wirth
Universität Münster
benedikt.wirth@uni-muenster.de

MS114

Conditions for the Holder Regularity of Local Minimizers of a Nonlinear Elastic Energy in Two Dimensions

We present conditions sufficient for the Holder regularity of minimizers of an energy which can model isotropic materials, including rubber. By hypothesizing that deformations u map circles to suitably star-shaped sets, and then by applying an adapted elliptic regularity theory, we can overcome some of the technical difficulties that have long been associated with proving regularity of elastic energy minimizers. A practical demonstration of the theory is given in the class of 'shear maps.

Jonathan J. Bevan
Department of Mathematics
University of Surrey
j.bevan@surrey.ac.uk

MS114

Multiscale Modeling of Rubber-Like Materials and Soft Tissues: *a Particular Perspective*

We survey, in a personal (and therefore *incomplete*) way, multiscale approaches for the modeling of rubber-like and soft tissues and compare them with classical macroscopic phenomenological models. Our aim is to show how it is possible to obtain feasible mathematical models of the mechanical behavior of these materials incorporating mesoscopic (network scale) informations. Multiscale approaches are crucial for a theoretical comprehension and prediction of the complex mechanical response of these materials. Moreover, such models are fundamental in the perspective of the design, via manipulation at the micro and nano scales, of new polymeric and bio-inspired materials with exceptional macroscopic properties.

Giuseppe Saccomandi
Università di Perugia
giuseppe.saccomandi@unipg.it

MS114

On the General Solution Based on the Time-Independent Integral, the Lagrangian and the Hamiltonian Functions for Fin Equation

We derive the time-independent integral for a nonlinear equation, namely fin equation in which the thermal conductivity and heat transfer coefficient are assumed to be functions of the temperature. Using the modified Prelle-Singer approach, we point out that explicit the time-independent first integral and general solution of the equation corresponding to these integrals can be identified for the fin equation for different thermal conductivity and heat transfer coefficient functions. Then using this approach, an appropriate the Lagrangian and the Hamiltonian forms are obtained. Finally, we discuss on these solutions by their graphics.

Teoman zer, zlem Orhan
Istanbul Technical University
tozer@itu.edu.tr, oorhan@itu.edu.tr

MS115

Solution Landscapes for Nematic Microfluidics

Abstract not available

Ian Griffiths
University of Oxford
griffit4@maths.ox.ac.uk

MS115

Linear Stability of Compressible Vortex Sheets in Elastodynamics

The linear stability of rectilinear compressible vortex sheets is studied for two-dimensional isentropic elastic flows. This problem has a free boundary and the boundary is characteristic. A necessary and sufficient condition is obtained for the linear stability of the rectilinear vortex sheets. A new approach of upper triangularization of the system is developed in the analysis. This is based on the joint work with Ming Chen and Dehua Wang.

Jilong Hu
University of Pittsburgh
jih62@pitt.edu

MS115

Global Existence and Finite Time Singularities for a Simplified Model of Liquid Crystal Flows

Abstract not available

Tao Huang
New York University-Shanghai
th79@nyu.edu

MS115

Flexible Colloidal Molecules: Lipid Ordering Reg-

ulated Bond Flexibility

The term colloidal molecule has been introduced to mark the similarity in shape and interactions between anisotropic colloidal particles and real molecules. This analogy does not extend, however, to intraparticle flexibility: colloidal particles are rigid objects, whereas real molecules are often flexible. I will here introduce assemblies of colloidal particles connected by strong, but mobile ball and socket joints by employing particles coated with mobile DNA linkers: flexible colloidal molecules. I will examine and quantify the various factors that influence the bond flexibility using particle tracking. Finally, I will demonstrate how these strong and specific, yet flexible bonds affect the assembly pathway and lead to structures with internal flexibility and unexpected symmetries.

Daniela J. Kraft
Leiden University, The Netherlands
kraft@physics.leidenuniv.nl

MS116

A Hybrid Numerical Method for Electrokinetic Flow with Deformable Interfaces

A hybrid or multiscale method is introduced to describe the evolution of either an immiscible fluid drop or a fluid-embedded vesicle in the two-phase flow of ionic fluids in the presence of an applied DC electric field. The starting point is the Poisson-Nernst-Planck equations in the Stokes flow regime, followed by their asymptotic reduction in the thin Debye layer limit. Current results and future modeling challenges will be discussed.

Michael R. Booty
Department of Mathematical Sciences, NJIT
booty@njit.edu

Michael Siegel
New Jersey Institute of Technology
misieg@njit.edu

MS116

An Accurate Metropolis-Hastings Algorithm and a Fast Multipole Method for Coarse-Grained Lipid Bilayer Membrane in Solvent

From empirical numerical verifications, using forward Euler scheme and the Fixman's scheme for Brownian dynamics simulations is not able to acquire the long-time accuracy and requires very small time steps. Our numerical studies show that the Metropolis adjusted Langevin algorithm (MALA) is adequate for running long-time Markov Chain Monte Carlo simulations, which are second order accurate. In this work, without explicitly calculating the interactions with fluid molecules, instead we simulate the coarse-grained dynamics of a lipid bilayer membrane in solvent using Rotne-Prague-Yamakawa tensor. We perform the velocity Verlet integration using the fast multipole method coupled with MALA, and observe the self-assembly property of membrane. We also extend the proposed algorithm to the simulations of shape transitions of both vesicle and a red blood cell.

Szu-Pei Fu, Shidong Jiang
Department of Mathematical Sciences
New Jersey Institute of Technology
sf47@njit.edu, shidong.jiang@njit.edu

Nawaf Bou-Rabee
Department of Mathematical Sciences
Rutgers UniversityCamden
nawafbourabee@me.com

Yuan-Nan Young
Department of Mathematical Sciences
NJIT
yyoung@njit.edu

Zhangli Peng
University of Notre Dame
zhangli.peng.15@nd.edu

Hongyan Yuan
University of Rhode Island
hongyan_yuan@uri.edu

MS116

Recent Advances in Modeling of Liposomes in Electric and Magnetic Fields

Vesicles undergo interesting dynamics when exposed to electric or magnetic fields. Electric fields induce large deformation in the vesicle membrane and alignment of vesicles in magnetic fields have also been demonstrated. Here, a recent numerical model of vesicles is presented that allows for the investigation of the electrohydrodynamics of mono- and multi-component vesicles in addition to the magneto-hydrodynamics of vesicles. The model, sample results, and possibilities for future work will be outlined.

David Salac, Prerna Gera
University at Buffalo - SUNY
davidsal@buffalo.edu, prernage@buffalo.edu

MS116

Computational Algorithms for Vesicle Electrohydrodynamics

In this talk, we discuss a new integral equation method for simulating the electrohydrodynamics of a suspension of vesicles. The classical Taylor-Melcher leaky-dielectric model is employed for the electric response of each vesicle and the Helfrich energy model combined with local inextensibility is employed for its elastic response. The coupled governing equations for the vesicle position and its transmembrane electric potential are solved using a numerical method that is spectrally accurate in space and first-order in time. The method uses a semi-implicit time-stepping scheme to overcome the numerical stiffness associated with the governing equations. We will present new results on the suspension rheology, two-body interactions and pattern formation. This is joint work with Bowei Wu.

Shravan Veerapaneni
Department of Mathematics
University of Michigan
shravan@umich.edu

MS117

Highly Accurate Methods for Resonance Calculations

Abstract not available

Nilima Nigam
Dept. of Mathematics

Simon Fraser University
nigam@math.sfu.ca

MS117

Novel Integral Formulations for Layered Media Problems in Electromagnetics

In this talk I will discuss recent developments in integral equation formulations of layered media scattering problems in electromagnetics, as well as new applications to problems in electrical engineering. In half-space or infinite planar geometries, integral equation methods must be augmented with image-based or local-Fourier methods in order to avoid discretization of unbounded regions. Various numerical techniques can then be used to obtain high-order solutions.

Michael O'Neil
New York University
oneil@cims.nyu.edu

MS117

Pathological Scattering of Electromagnetic Waves in Magneto-Photonic Crystals with Defects in the Slow-Light Regime

In this talk, I will discuss a new type of slow-wave phenomenon in magneto-photonic crystals (MPCs) associated with a defect layer and frozen (stopped) light. A perturbation analysis is given of the scattering problem of incident fields in a MPC by the defect layer near a stationary inflection point of the dispersion relation. Scattering is pathological especially in the presence of a "frozen-light defect mode" and this will be the focus of this talk.

Aaron T. Welters
Department of Mathematical Sciences
Florida Institute of Technology
awelters@fit.edu

Shipman Shipman
Louisiana State University
shipman@math.lsu.edu

MS118

Regularity and Related Properties for Minimizers of Maier-Saupe Energies for Liquid Crystals

We discuss regularity results for Maier-Saupe energies used to characterize nematic liquid crystal configurations. The energy density is singular, as in Ball and Majumdar's modification of the Landau-de Gennes Q-tensor model, so as to constrain the competing states to take values in the closure of a physically realistic range. We prove that minimizers are regular and in several model problems this implies that minimizers take on values strictly within the physical range.

Patricia Bauman
Purdue University
bauman@math.purdue.edu

MS118

Liquid Crystal Electrokinetics

We consider flow of liquid crystals containing ionic charges and driven by an applied electric field. Recent experiments show remarkable new features resulting from coupling between flow anisotropy, especially defects, and electric charge [O.D.Lavrentovich, 2014]. We present the Ericksen-Leslie equations of electrokinetics and discuss their well-posedness. We give examples of charge separation in connection with line defects in Poiseuille flow. The research is aimed at understanding phenomena of nonlinear electrophoresis in liquid crystal flow environment.

Maria-Carme Calderer
Deparment of Mathematics
University of Minnesota, USA
calde014@umn.edu

MS118

Theory and Experiments of Topologically Driven Flows in Nematic Suspensions

We present theory, numerical solutions, and experiments of electric field driven flows in nematic liquid crystals (LC) in which a patterned molecular orientation acts as an electrolytic active medium. Surface patterning by photoalignment in a thin cell is used to create various alignments of a nematic liquid crystal film, that may include topological defects. The active patterned LC electrolyte converts electric field energy into LC flows and transport of embedded particles of any type (fluid, solid, gaseous) along predesigned trajectories, and without limitation on the electric nature (charge, polarizability) of these particles and interfaces. Flow is quadratic in the electric field which leads, even for an imposed AC field, to systematic flow velocities, including persistent vortices of controllable rotation speed and direction. The latter are essential for micro- and nanoscale mixing applications.

Jorge Vinals
School of Physics and Astronomy
University of Minnesota
vinals@umn.edu

MS118

Mean Field Models for Lyotropic Nematic Liquid Crystals

It is an interesting challenge in statistical physics and PDE to be able to connect models for the evolution of particles with macroscopic equations which describe their 'average' behaviour. We shall be interested in systems of lyotropic nematic liquid crystals. Indeed, beginning with a model for N interacting hard (or soft) ellipsoids embedded in an ambient fluid, we investigate its mean field limit as N diverges in order to recover a coupled PDE system for the evolution of a distribution function (modelling the average behaviour of the particles) coupled with a fluid equation (which governs the evolution of the ambient fluid). We shall discuss some results on some relatively simple particle regimes.

Mark Wilkinson
Courant Institute
mwilkins@cims.nyu.edu

MS119

On the Connection Between Dislocation Mechanics and Continuum Crystal Plasticity

We show how the structure of classical crystal plasticity theory is a natural averaged picture of microscopic, time-dependent, dislocation dynamics, stated in the language of nonlinear partial differential equations. Both the microscopic and meso-macroscopic models will be illustrated

with selected results. We will outline one set of questions directed towards deriving constitutive equations for the averaged macroscopic model described above and, time permitting, describe our present efforts in that direction.

Amit Acharya
Civil and Environmental Engineering
Carnegie Mellon University
acharyaamit@cmu.edu

Xiaohan Zhang
Stanford University
xiaohanzhang.cmu@gmail.com

Saurabh Puri
Simulia, Inc.
saurabhpuri2005@gmail.com

MS119

Capturing the Stochastic Behavior of Nanoindentation Pop-In with Dislocation Dynamics

Session code: AF; oral; Yes, can transfer to poster. Nanoindention experiments on materials with high dislocation densities demonstrate a stochastic pop-in force due to the activation of pre-existing dislocations, rather than dislocation nucleation. In the present work, we have developed a coupled finite element - discrete dislocation dynamics simulator to identify the underlying mechanisms that lead to pop-in. Multiple random dislocation configurations and several dislocation densities are simulated and the resulting cumulative distribution functions for pop-in are compared to simpler stochastic models.

Joshua C. Crone
US Army Research Laboratory
joshua.crone.civ@mail.mil

Lynn B. Munday
Army Research Lab
lynn.b.munday.civ@mail.mil

Jaroslaw Knap
U.S. Army Research Laboratory
jaroslaw.knap.civ@mail.mil

MS119

Thermodynamically Consistent Continuum Dislocation Dynamics

Continuum dislocation dynamics (CDD) provides kinematically consistent evolution equations of dislocation alignment tensors, presuming a given average dislocation velocity (Hochrainer (2015), Philos. Mag. 95 (12), 1321–1367). In the current work we demonstrate how a free energy formulation may be used to derive constitutive equations for the dislocation velocity. We validate the theory via numerical comparisons of CDD simulations with discrete dislocation simulations of small scale plasticity.

Thomas Hochrainer
University of Bremen
Bremer Institut für Strukturmechanik und Produktionsanlagen
hochrain@uni-bremen.de

Alireza Ebrahimi
Universitat Bremen
ebrahimi@uni-bremen.de

MS120

Modeling and Simulation for Solid-State Dewetting Problems

In this talk, I will present sharp interface models with anistropic surface energy and a phase field model for simulating solid-state dewetting and the morphological evolution of patterned islands on a substrate. The sharp interface model tracks the moving interface explicitly and it is very easy to be handled in two dimensions via arclength parametrization. The phase field model is governed by the Cahn-Hilliard equation with isotropic surface tension and variable scalar mobility and it easily deals with the complex boundary conditions and/or complicated geometry arising in the solid-state dewetting problem. Since the phase field model does not explicitly track the moving surface, it naturally captures the topological changes that occur during film/island morphology evolution. Efficient and accurate numerical methods for both sharp interface models and phase field models are proposed. They are applied to study numerically different setups of solid-state dewetting including short and long island films, pinch-off, hole dynamics, semi-infinite film, etc. Our results agree with experimental results very well. This is joint works with Wei Jiang, David J. Srolovitz, Carl V. Thompson, Yan Wang and Quan Zhao.

Weizhu Bao
National University of Singapore
Department of Mathematics
matbaowz@nus.edu.sg

MS120

Sharp-Interface Models for Solid-State Dewetting Problems

Based on a thermodynamical variational approach, we propose sharp-interface models for simulating solid-state dewetting of thin films with anisotropic surface energies. The morphology evolution of thin films is governed by surface diffusion and contact line migration. For the contact line migration, we introduce a relaxation kinetics with a finite contact line mobility by energy gradient flow method. By using the proposed models, we investigate the anisotropy effects on thin solid film dewetting. Especially, we show that when the surface energy anisotropy is strong, multiple equilibrium shapes may appear which can not be described by the classical Winterbottom construction. We repair the Winterbottom construction to include multiple equilibrium shapes and employ our model to demonstrate that all such shapes are dynamically accessible.

Wei Jiang
Wuhan University and National University of Singapore
jiangwei1007@whu.edu.cn

MS120

Solid State Dewetting on Curved Substrates

We consider the case of the evolution of a discontinuous film on arbitrarily curved, rigid substrates, for both isotropic and anisotropic surface energies. The model is derived for sharp interfaces and includes dynamic wetting angles. We implement the model in a parametric finite element method and apply it to both small and large islands on both smoothly curved substrates as well as substrates

with sharp features and to the case of template dewetting.

David J. Srolovitz
University of Pennsylvania
srol@seas.upenn.edu

Yan Wang
National University of Singapore
a0086260@u.nus.edu

Wei Jiang
Wuhan University and National University of Singapore
jiangwei1007@whu.edu.cn

Weizhu Bao
National University of Singapore
Department of Mathematics
matbaowz@nus.edu.sg

MS120

Nanostructure Formation via Template-Guided Dewetting

Solid state dewetting (SSD) of a metal film on a patterned substrate has received renewed attention recently, due to its ability to control the size and location of produced metallic nanostructures. Although the SSD technique has been used to fabricate various regular arrays, such as nanodots,nano-apertures, nanowires and nanorods, all these nanostructures were obtained to a large degree by trial and error. Since the film thickness and the geometry of the substrate exert great influence on the dewetted thin film morphologies, it is thus both important and necessary to understand the dewetting mechanisms and map out phase diagrams so as to provide robust theoretical guidelines for their fabrication with high precision. We perform systematic energetic analyses and phase field simulations to study the stability of various nanostructures formed by dewetting of solid metal films deposited on patterned substrates. Phase diagrams are presented to show the complex relations between those system parameters and various nanostructure morphologies. The phase diagrams we have obtained provide clear guidelines for using solid-state dewetting as a tool to achieve various nanostructure arrays.

Yong-Wei Zhang
Institute of High Performance Computing, Singapore
zhangyw@ihpc.a-star.edu.sg

Liangxing Lu
Institute of High Performance Computing
Institute of High Performance Computing
lul@ihpc.a-star.edu.sg

Bharathi Srinivasan
Institute of High Performance Computing, Singapore
srinivasan@ihpc.a-star.edu.sg

Yingmin Wang, Mohamed Asbahi, Joel Yang
Institute of Materials and Research Engineering, Singapore
wangym@imre.a-star.edu.sg, asbahim@imre.a-star.edu.sg, joel_yang@sutd.edu.sg

MS121

Inverse Problems for the Schrödinger and Conductivity Problems on Networks

We consider the problem of finding the electric properties of components in an electric circuit from measurements made at a few nodes. We give a condition based on the linearization of the problem that is sufficient to guarantee that the problem has a unique solution, except for a zero measure set. Our approach borrows ideas from the Complex Geometric Optics method that has been used to show uniqueness for continuum inverse problems.

Fernando Guevara Vasquez
University of Utah
fguevara@math.utah.edu

MS121

Soret Effects in Electrokinetically-Driven Heat Exchangers for Electronics Applications.

We extended classical asymptotic approaches to allow for the spatial pattern wavenumber to vary on the macroscale variables and to find how changes in microstructure geometry affect macroscopic properties and transport. We consider here the thermal transport of a weakly dielectric coolant through nonuniformly spaced laminates, under an applied electric field, as a simple model for heat sinks in electronics. Power is continuously being generated by the laminates, and the local rates of heat and ion transport depend on the local electric potential, local ion concentrations, and local thermal gradients in the coolant. We find a coupled system of pdes that describe the local microscale temperature and deviations from the Darcy pressure. Microscale values of all of these quantities are known in terms of the solutions to these effective equations.

Silvia Jimenez Bolanos
Department of Mathematics
Colgate University
sjimenez@colgate.edu

Burt S. Tilley
Worcester Polytechnic Institute
Mathematical Sciences Department
tilley@wpi.edu

Bogdan M. Vernescu
Worcester Polytechnic Inst
Dept of Mathematical Sciences
vernescu@wpi.edu

MS121

Spectral Analysis and Computation of Effective Diffusivities for Steady Random Flows

a) Minisymposium Session Code: MS16 b) ORAL c) NO The long time, large scale behavior of advection-diffusion of passive tracers by random flows is equivalent to an enhanced diffusive process with an effective diffusivity tensor D^*. We will discuss Stieltjes integral representations for D^*, involving the spectral measure μ of a self-adjoint random operator. We will also present rigorous methods for computing μ, formulated in terms of eigenvalues and eigenvectors of random matrices. Results will be viewed through the lens of random matrix theory.

N. Benjamin Murphy
University of Utah
murphy@math.utah.edu

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

Jingyi Zhu
Department of Mathematics
University of Utah
zhu@math.utah.edu

Jack Xin
Department of Mathematics
UCI
jxin@math.uci.edu

Kenneth M. Golden
University of Utah
golden@math.utah.edu

MS121

Fast Algorithm for Computing Effective Properties of Two-Phase Composites

The focus of this talk is on implementation of fast algorithms for computing the effective static properties of two-phase composite materials in 3D with geometry defined by micro-CT scans. To generate surface mesh of samples with complicated geometry such as trabecular bone, several crucial modifications to the open source code *surfacemesh* (developed by P.-O. Persson) will be explained and demonstrated in this talk. BEM-FMM computation using the resulting mesh will be given as well.

Miao-Jung Y. Ou
University of Delaware, USA
Department of Mathematical Sciences
mou@udel.edu

Y.-H. Richard Tsai
Department of Mathematics
University of Texas at Austin
ytsai@math.utexas.edu

Wai-Yip Chan
Chinese University of Hong Kong
wai-wai123@hotmail.com

Seong Jun Kim
Georgia Institute of Technology
skim396@math.gatech.edu

MS122

Rigid Multiblob Models of Suspensions of Rigid Particles of Complex Shapes in Confinement

I will discuss computational methods for problems involving Brownian rigid and semi-rigid particles immersed in a fluid. There are a number of methods developed for suspensions of spheres at small Reynolds numbers, such as the well-known method of Stokesian Dynamics, or boundary-integral formulations. More complex rigid bodies suspended in fluid can be represented with different degrees of fidelity by enforcing a rigidity constraint on a collection of blobs resolving the body to some degree of fidelity. Implementing all of this in practice efficiently for suspensions of tens of thousands of particles is possible but requires some sophisticated numerical linear algebra which I will discuss in some detail. Thermal fluctuations and thus Brownian motion can be consistently modeled by including a fluctuating (random) stress in the momentum equation, as dictated by fluctuating hydrodynamics.

Aleksandar Donev
Courant Institute of Mathematical Sciences
New York University
donev@courant.nyu.edu

MS122

Immersed Particle Dynamics in Fluctuating Fluids with Memory

We present a fluctuating Stokes model for an immersed particle passively advected by a Maxwellian fluid via the inclusion of the memory's correlations in a thermal stress. We describe the resulting stochastic partial differential equations for the non-Markovian, stationary fluid velocity process and we present a covariance based numerical method for generating particle paths. Finally, we apply standard experimental one-point microrheology protocol to recover bulk loss and storage modulus and quantify the resulting errors.

Christel Hohenegger
University of Utah
Department of Mathematics
choheneg@math.utah.edu

Scott McKinley
University of Florida
scott.mckinley@ufl.edu

MS122

Frictional Interactions in Viscous Suspensions: Discontinuous Shear Thickening and Shear Jamming

Discontinuous shear thickening (DST) observed in many dense athermal suspensions has proven difficult to understand and to reproduce by numerical simulation. By introducing a numerical scheme including both relevant hydrodynamic interactions and granularlike contacts, we show that contact friction is essential for having DST. Above a critical volume fraction, we observe the existence of two states: a low viscosity, contactless (hence, frictionless) state, and a high viscosity frictional shear jammed state. These two states are separated by a critical shear stress, associated with a critical shear rate where DST occurs. The shear jammed state is reminiscent of the jamming phase of granular matter. Continuous shear thickening is seen as a lower volume fraction vestige of the jamming transition.

Jeffrey Morris
Levich Institute
City College of NY, CUNY
morris@ccny.cuny.edu

MS122

Modeling the Effect of Hydrophobicity on Nanoparticle Suspensions

Modeling suspensions of particles at the nanoscale requires numerical approaches that are essentially different from those developed for microscopic systems. There is not an adequate method, for instance, to describe the hydrophobic collapse of nanoparticles at scales that are not accessible by traditional molecular dynamics simulations. In this talk

I will present a new fluctuating hydrodynamics based approach that describes adequately wetting-dewetting transitions during the hydrophobic collapse and discuss how this phenomenon could affect suspensions of nanoparticles.

Nikolaos Voulgarakis
Washington State University
nvoul@math.wsu.edu

MS123

Large Motions of Nonlinearly Viscoelastic Rods and Shells

This lecture surveys recent results on steady states and motions of nonlinearly viscoelastic rods and shells subject to live loads (such as hydrostatic pressure, centrifugal force, and stick-slip friction). The special emphasis given to the interaction of geometrically exact formulations, the compatible use of general constitutive equations for material response, and the presence of live loads shows how these factors play crucial roles in the behavior of solutions.

Stuart S. Antman
Dept of Mathematics, Inst. Phys. Sci & Tech, Inst. Systems R
UMCP
ssa@math.umd.edu

Alexey Stepanov
University of Maryland
alex314@umd.edu

Suleyman Ulusoy
Zirve University
suleyman.ulusoy@zirve.edu.tr

MS123

A Model For Dislocations In Epitaxially Strained Elastic Films

We present a variational model for nucleation of dislocations in epitaxially strained films. This is joint work with Nicola Fusco, Irene Fonseca, and Massimiliano Morini.

Giovanni Leoni
Carnegie Mellon University
giovanni@andrew.cmu.edu

MS123

On a Variational Model for the Elasticity of Biomembranes

Biomembranes are remarkable structures with both fluid-like and solid-like properties: the main constituents are amphiphilic lipids, which have a head part that attracts water and a tail part that repels it. Because of these properties, such lipids organize themselves in micelle and bilayer structures, where the head parts shield the lipid tails from the contact with water. In a recent paper by Peletier and Röger (Arch. Rational Mech. Anal. 2009) a mesoscale model was introduced in the form of an energy for idealized and rescaled head and tails densities: the energy has two contributions, one penalizes the proximity of tail to polar (head or water) particles and the second implements the head-tail connection as an energetic penalization. The tickness of the structure is very small, and a full Gamma-convergence result has been proved in the same paper in the two-dimensional case: the Gamma-limit turns out to be the Euler elasitca functional for curves in the plane. The three-dimensional case is much harder and we have only partial results. In this seminar I will present the mesoscopic model proposed by Peletier and Röger, I will briefly explain how the deduction of the 2D-macroscopic model by Gamma-convergence works and then I will give some details on the 3D-case: the analysis of such a case requires deep tools from geometric measure theory, like currents and varifolds, in order to have weak notions of surfaces good for Calculus of Variations and for which a suitable notion of curvatures exists. The research project is in collaboration with Mark Peletier and Matthias Röger.

Luca Lussardi
Università Cattolica del Sacro Cuore
luca.lussardi@unicatt.it

MS123

Island Formation in Epitaxially Strained Films

We consider variational models for epitaxially strained crystalline films on rigid substrates. The associated energy functional accounts for the elastic strain energy due to a crystallographic mismatch between the substrate and the film, and the surface energy of the film's free surface. Mathematically the energy can be viewed as a nonlocal isoperimetric functional. We study existence of minimizers in dependence on various problem parameters.

Barbara Zwicknagl
University of Bonn
zwicknagl@iam.uni-bonn.de

MS124

Isotropic-Nematic Phase Transitions in Elastic Rigid Rod Newtorks

We study isotropic-nematic phase transitions in a system consisting of an elastic network with rigid rods. We observe that such transitions are driven by, the relative size of the rod length and network strands; the rod density and aspect ratio. Our constitutive theory is developed upon the lyotropic liquid crystal elastomers. We compare our results with molecular simulations for actin systems.

Carlos A. Garavito Garzon, Carme Calderer
University of Minnesota
garav007@umn.edu, calde014@umn.edu

MS124

Fractional Modeling of Viscoelasticity in Cerebral Arteries and Aneurysms

We developed effective numerical methods for fractional-order PDEs to investigate viscoelastic aneurysm wall models, by combining a fast convolution method with the high-order BDF. We confirmed that comparing with the integer-order models, the fractional-order models are less sensitive to the relaxation parameters. In patient-specific aneurysm studies, we developed a fractional-order aneurysm wall model from the loading test. More realistic deformation distribution is observed for this model when comparing against the results from healthy arterial configurations.

Yue Yu
Department of Mathematics, Lehigh University
yuy214@lehigh.edu

Paris Perdikaris

Massachusetts Institute of Technology
parisp@mit.edu

George Em Karniadakis
Brown University
george_karniadakis@brown.edu

MS125

Defect Behaviors of Liquid Crystals on a Spherical Surface: A Self-consistent Field Theory Simulation

We consider the system when liquid crystals are confined on the spherical surface. Due to the spatial frustration, many defect patterns with discontinuity in the orientation of molecules can be formed. In this work, we studied the impact of molecule length, sphere radius, density and rigidity of polymers on the pattern. A new pseudo-spectral method is designed to solve the corresponding self-consistent field theory equations. Results of this molecule-level simulation are consistent with fommer experimental or theoretical work.

Qin Liang
Xiangtan University, China
liangqin1997@xtu.edu.cn

MS125

On the Local Controllability of Nematic Liquid Crystal Flow

Abstract not available

Yuning Liu
NYU-Shanghai
yl67@nyu.edu

MS125

Front Propagation for Nematic Liquid Crystals

Abstract not available

Apala Majumdar
University of Bath
a.majumdar@bath.ac.uk

MS126

Multiscale Modeling of Mechanosensing Channels on Vesicles and Cell Membranes in 3D Constricted Flows and Shear Flows

We apply a multiscale approach to investigate the gating of mechanosensitive channels on vesicles and cell membranes under different flow conditions. At the cell level (microns), the membrane tension is calculated using a 3D two-component whole-cell membrane model based on dissipative particle dynamics (DPD), including the cortex cytoskeleton and its interactions with the lipid bilayer. At the mechanosensitive channel level (nanometers), we predict the relation between channel gating and the membrane tension obtained from a cell-level model using a semi-analytical model based on the bilayer hydrophobic mismatch energy. We systematically study the gating of channels of vesicles and cell membranes in constricted channel flows and shear flows, and explore the dependence of the gating on flow rate, cell shape and size. The results provide guidance for future experiments in inducing mechanosensitive channel opening for various purposes such as drug delivery.

Zhangli Peng, Zhangli Peng
University of Notre Dame
zhangli.peng.15@nd.edu, zpeng3@nd.edu

On Shun Pak
Santa Clara University
opak@scu.edu

Yuan-Nan Young
Department of Mathematical Sciences
NJIT
yyoung@njit.edu

MS126

Complex Viscoelasticity of Shape Changes and Surface Hydrodynamics of Membrane Protrusions

Cell membranes are confined and dynamically go out of equilibrium by localized forces. We experimentally and computationally study the membrane shape dynamics in bio-mimetic conditions, such as the formation of protrusions from confined lipid bilayers upon contraction, and also dynamical membrane invaginations upon the PH-induced, localized lipid packing. We formulate and numerically implement a dynamical continuum model that is nonlinear, and allows general shapes. Our model describes the coupled shape dynamics, lipid hydrodynamics and interlayer slippage.

Mohammad Rahimi
Princeton University
rahimi@princeton.edu

Marino Arroyo
Universitat Politecnica de Catalunya
marino.arroyo@upc.edu

Margarita Staykova
Durhan University
margarita.staykova@durham.ac.uk

Howard A. Stone
Mechanical and Aerospace Engineering
Princeton University
hastone@princeton.edu

MS126

Fluctuation and Dynamics of a Lipid Bilayer Membrane Under an Electric Field

Membrane fluctuation and dynamics under an electric field is investigated, and results show that the membrane instability and dynamics depend not only on the mismatch in conductivity and permittivity between the bulk fluids, but also on the membrane charging time. In addition, the (entropic) membrane tension is found to depend on the electric field. Lubrication theory is utilized to examine the nonlinear dynamics of a planar lipid bilayer membrane with and without electrokinetics.

Yuan-Nan Young
Department of Mathematical Sciences, NJIT
yyoung@njit.edu

M.J. Miksis
Engineering Science and Applied Mathematics

Northwestern University
m-miksis@northwestern.edu

MS126

Deformation-Relaxation of Vesicles

Deformation-based techniques have played an important role in mechanical analysis of vesicles, cells, and other biological tissues. On the other hand, shape relaxation upon release of deforming force is found to exhibit behavior that reveals key physical mechanisms, and is amenable to analytical solution strategies. Here such results are presented which demonstrate similarity, regime separation, and agreement between theoretical solution and experimental data.

Miao Yu
Rutgers, The State University of New Jersey
Mechanical and Aerospace Engineering Department
miaoyu@rutgers.edu

Rafael Lira
Max Planck Institute of Colloids and Interfaces
Department of Theory and Bio-Systems
rafael.lira@mpikg.mpg.de

Karin Riske
Universidade Federal de São Paulo
Departamento de Biofsica
kar@if.usp.br

Rumiana Dimova
Max Planck Institute of Colloids and Interfaces
Department of Theory and Bio-Systems
rumiana.dimova@mpikg.mpg.de

Hao Lin
Department of Mechanical and Aerospace, Rutgers University
hlin@jove.rutgers.edu

MS127

Mechanism of Absorption Suppression in Gyroscopic Systems Composed of High-Loss and Lossless Components

In this talk, I will discuss the development of a theory of broadband absorption suppression in magnetic composites. Using a Lagrangian framework, we introduce a model for two-component linear systems with a high-loss and a lossless component in order to study the interplay of dissipation and gyroscopy as well as the dominant mechanisms of energy loss. New results are discussed related to modal dichotomy and selective overdamping phenomena in gyroscopic-dissipative systems.

Alexander Figotin
Department of Mathematics
University of California at Irvine
afigotin@uci.edu

Aaron T. Welters
Department of Mathematical Sciences
Florida Institute of Technology
awelters@fit.edu

MS127

Effective Properties of Periodic Tubular Structures

A method is described to calculate effective tensor properties of a periodic array of two-phase dielectric tubes embedded in a host matrix. The method uses Weierstrass' zeta-functions for representation of the potential that considerably facilitates the problem and allows us to find an exact expression for the effective tensor. We also discuss dependence of the effective tensor on the frequency of the external field.

Yuri Godin
University of North Carolina at Charlotte
ygodin@uncc.edu

MS127

Electric Quadrupolarizability of a Source-Driven Dielectric Sphere

Since both metamaterials comprised of artificial molecules and natural molecular materials at optical and greater frequencies can exhibit significant electric quadrupolarization as well as electric and magnetic dipolarization, we determine the passive, causal electric quadrupolarizability for a spherically symmetric molecule, namely a dielectric sphere subject to source-driven applied fields. For source-free fields, such as the fields of the eigenmodes of an electric quadrupolar array, the local electric field illuminating each inclusion is solenoidal, the constitutive relation is characterized by just one quadrupolarizability constant (rather than two in the source-driven case), and the electric quadrupolarization becomes traceless.

Arthur D. Yaghjian
Electromagnetics Research Consultant
Concord, MA 01742 USA
a.yagjhian@comcast.net

MS128

Exotic New Phases in Confined Chiral Liquid Crystals

The thermodynamic state of chiral liquid crystals in nano confined geometries is obtained from a theoretically informed Monte Carlo relaxation of the tensor alignment field Q. The free energy of the system is described in the framework of the Landau-de Gennes formalism, including the isotropic-nematic, the elastic and the surface free energy densities. Our approach allows the treatment of highly chiral systems in complex geometries without the common one-elastic constant approximation. Anchoring strength, curvature and chirality are explored in multiple scenarios, providing a complete understanding of the energy landscapes. Previously known phases, such as twist bipolar (BS), radial spherical structure (RSS), twist cylinder (TC), double twist cylinder (DTC) and blue phases (I, II and III), are observed and characterized in terms of the elastic distortions and the free energy penalizations at the surface. For highly chiral liquid crystals in non-spherical cavities, the disclination lines are twisted or bent near the surfaces preventing the formation of symmetric networks of defects. Finally, specific ratios of confinement and curvature, for cylindrical and toroidal cavities, give rise to novel phases including a double helix blue phase.

Juan Hernandez-Ortiz

Universidad Nacional de Colombia, Sede Medellin
jphernandezo@wisc.edu

MS128

A Finite Element Method for Nematic Liquid Crystals with Variable Degree of Orientation

We consider the simplest one-constant model, put forward by J. Ericksen, for nematic liquid crystals with variable degree of orientation. The equilibrium state is described by a director field n and its degree of orientation s, where the pair (s, n) minimizes a sum of Frank-like energies and a double well potential. In particular, the Euler-Lagrange equations for the minimizer contain a degenerate elliptic equation for n, which allows for line and plane defects to have finite energy. We present a structure preserving discretization of the liquid crystal energy with piecewise linear finite elements that can handle the degenerate elliptic part without regularization, and show that it is consistent and stable. We prove Γ-convergence of discrete global minimizers to continuous ones as the mesh size goes to zero. We develop a quasi-gradient flow scheme for computing discrete equilibrium solutions and prove it has a strictly monotone energy decreasing property. We present simulations in two and three dimensions to illustrate the method's ability to handle non-trivial defects.

Ricardo Nochetto
Department of Mathematics
University of Maryland, College Park
rhn@math.umd.edu

Shawn W. Walker
Louisiana State University
Department of Mathematics and CCT
walker@math.lsu.edu

Wujun Zhang
University of Maryland
wujun@umd.edu

MS128

Numerical Approximation of the Ericksen Leslie Equations

The Ericksen Leslie equations model the motion of nematic liquid crystaline fluids. The equations comprise the linear and angular momentum equations with non-convex constraints on the kinematic variables. These equations possess a Hamiltonian structure which reveals the subtle coupling of the two equations, and a delicate balance between inertia, transport, and dissipation. While a complete theory for the full nonlinear system is not yet available, many interesting sub-cases have been analyzed. This talk will focus on the development and analysis of numerical schemes which inherit the Hamiltonian structure, and hence stability, of the continuous problem. In certain situations compactness properties of the discrete solutions can be established which guarantee convergence of schemes.

Noel J. Walkington
Department of Mathematical Sciences
Carnegie Mellon University
noelw@andrew.cmu.edu

MS128

Computational Modeling of Tactoid Dynamics in Chromonic Liquid Crystals

The Isotropic-nematic phase transition in chromonic liquid crystals is studied, motivated by recent experiments. During temperature decrease, nematic nuclei nucleate, grow, and coalesce, giving rise to tactoid microstructures in an isotropic liquid. These tactoids produce topological defects at domain junctions (disclinations in the bulk or point defects on the surface). We simulate such tactoid equilibria and dynamics with a model using degree of order and a variable length director as state descriptors.

Chiqun Zhang
Canegie Mellon University
chiqunz@andrew.cmu.edu

Noel J. Walkington
Department of Mathematical Sciences
Carnegie Mellon University
noelw@andrew.cmu.edu

Amit Acharya
Civil and Environmental Engineering
Carnegie Mellon University
acharyaamit@cmu.edu

Oleg Lavrentovich
Kent State University
olavrent@kent.edu

MS129

Accounting for the Effect of Dislocations in Continuum Plasticity by Means of a Non-Local Spectral Formulation

We present the numerical implementation of a non-local polycrystal plasticity theory using a spectral formulation. Numerical procedures for the accurate estimation of higher-order derivatives of micromechanical fields are identified and applied. The new formulation is first used to solve a periodic laminate made of two crystals to assess the soundness and stability of the proposed algorithm, and next applied to 3-D fcc polycrystals, illustrating the computation of meaningful solutions of large problems in reasonable times.

Ricardo Lebensohn
Los Alamos National Laboratory
lebenso@lanl.gov

Alan Needleman
Texas A&M University
needle.tamu@gmail.com

MS129

Modeling the Annealing of Thin Films on Lattice-Mismatched Substrates with Discrete Dislocation Dynamics

In principle, discrete dislocation dynamics (DDD) may be used to model the annealing of a thin film overlaying a substrate. The practice, however, is complicated by approximations of the film/substrate interface, as well as the computational expense entailed by the tracking of dislocations, which can limit the time scale practically achievable by a DDD simulation. The advantages and disadvantages of the DDD approach as compared with other simplified

approaches will be discussed.

James J. Ramsey
Army Research Laboratory
james.j.ramsey14.civ@mail.mil

MS129

Homogenization of Dislocation Interactions in Regions of High Stress Concentrations

A self-consistent coarsening of dislocation interactions is discussed in the context of a dislocation based continuum model. In order to construct an efficient numerical implementation, several issues have to be resolved including the calculation of the stress field of a system of dislocations, dislocation correlation, and boundary conditions. Using the comparison with discrete dislocation dynamics in a few simple systems, the multi-component stress field which must be considered for dislocation density motion is discussed and enhanced by a statistical model for the representation of dipole interactions in the continuum formulation.

Katrin Schulz
Karlsruhe Institute of Technology
katrin.schulz@kit.edu

MS129

An A/C Study for Nano-Indentation and Homogeneous Dislocation Nucleation

Abstract not available

Lei Zhang
Shanghai Jiao Tong University
lzhang2012@sjtu.edu.cn

MS130

Modeling and Simulation of Moving Contact Lines in Multi-Phase Fluids

The moving contact line problem is a classical problem in fluid mechanics. The difficulty stems from the fact that the classical Navier-Stokes equation with no-slip boundary condition predicts a non-physical singularity at the contact line with infinite rate of energy dissipation. In this talk, we will discuss how the continuum theory, molecular dynamics and the more recently developed multiscale techniques can be combined to give us a better understanding of the fundamental physics of the moving contact line and formulate simple and effective models. We also illustrate how this model can be used to analyze the behavior of the apparent contact angle, hysteresis and other important physical problems for the moving contact line.

Weiqing Ren
National University of Singapore and IHPC, A-Star
matrw@nus.edu.sg

MS130

The Dynamics of Three-Phase Triple Junction and Contact Line

A projection approach is proposed for the derivation of a consistent free energy functional for the three-phase Cahn-Hilliard equations. The system is then coupled with the Navier-Stokes equations to describe the three-phase flow on solid surface with moving contact line. We show some numerical results for the dynamics of triple junction and four phase contact line. We also study the sharp interface limit of the three component Cahn-Hilliard system. The dynamic laws for the interfaces, the triple junctions and the contact points are derived at different time scales.

Xiaoping Wang
Hong Kong University of Science and Technology
mawang@ust.hk

MS130

Modified Wenzel and Cassie Equations for Wetting on Rough Surfaces

Wetting on rough surfaces is common in nature and industrial applications. The classical Wenzels and Cassies equations are widely used to characterize apparent contact angles of a liquid drop on these surfaces. However, the two equations can not describe the contact angle hysteresis phenomenon, which is often observed in reality. I will talk about our recent analysis for this problem. We derive some modified Wenzels and Cassies equations by homogenization method, that are consistent with experimental observations.

Xianmin Xu
Chinese Academy of Sciences
and RWTH Aachen University
xmxu@lsec.cc.ac.cn

Xiaoping Wang
Hong Kong University of Science and Technology
mawang@ust.hk

MS130

Modeling and Simulation of Moving Contact Line Problem for Two-Phase Complex Fluids Flow

We introduce a sharp interface continuum model for moving contact lines with insoluble surfactants. The interface and boundary conditions are derived from the consideration of energy dissipations. A finite element numerical method is developed to solve the coupled partial differential equations. Numerical experiments are presented for the model validation. We also discuss the model reduction of the slip model to the no-slip limit by the technique of asymptotic analysis.

Zhen Zhang
South University of Science and technology of China
zhangz@sustc.edu.cn

Weiqing Ren
National University of Singapore and IHPC, A-Star
matrw@nus.edu.sg

MS131

Optimal Structures of Three-Dimensional Composites

We describe new types of 3d optimal structures composed from three materials that satisfy the HashinShtrikman or Translation bounds and are realizable in a larger set of parameters than previously known optimal structures. One type is a multiscale structure a 3d analog of GibianskySigmund 2d optimal composite. The second type is a structure obtained by applying an optimal control approach to the differential scheme. We conject optimal structures for the

remaining range of parameters.

Andrej V. Cherkaev
Department of Mathematics
University of Utah
cherk@math.utah.edu

MS131

Exact Relations and Links for Fiber-Reinforced Elastic Composites

In the context of fiber-reinforced elastic composites there are many special situations where certain combinations of effective moduli can be expressed in terms of the properties of the constituent materials *regardless of the microstructure*. There are even more cases where we can relate effective tensors of two composites with the same, but otherwise *arbitrary* microstructure. I will describe the body of work that has culminated in the list of all such microstructure-independent formulas.

Yury Grabovsky
Temple University
yury@temple.edu

MS131

Mesoscopic Modeling of Active Suspensions

Starting from a fine-scale dissipative particle dynamics (DPD) model of self-motile point particles, we derive mesoscale continuum equations by applying a spatial averaging version of the Irving–Kirkwood–Noll procedure. The resulting stochastic continuum theory is similar to the well known theory of Toner and Tu. However, our theory also involves a constitutive equation for the average fluctuation force, according to which the strength and the probability distribution of this force vary with time and position. Although the fine scale self-propulsion force contains no explicit mechanism for aligning the velocities of neighboring DPD particles, the averaged coarse-scale equations include the commonly encountered cubically nonlinear body force density.

Alexander Panchenko
Washington State University
panchenko@math.wsu.edu

MS131

Discrete Breathers in a Resonant Granular Chain

We study a locally resonant granular material in the form of a Hertzian chain with linear internal resonators. Using an asymptotic reduction to a modified version of the discrete p-Schrödinger equation, we show that the system admits dark-breather solutions: exponentially localized, time-periodic states mounted on top of a non-vanishing background. A feature distinguishing our results from other settings where dark breathers are observed is the complete *absence* of a linear spectral band in the system.

Lifeng Liu
Department of Mathematics
University of Pittsburgh
lifengliu1104@gmail.com

Guillaume James
INRIA - Rhône Alpes
guillaume.james@inria.fr

Panayotis Kevrekidis
University of Massachusetts
kevrekid@math.umass.edu

Anna Vainchtein
Department of Mathematics
University of Pittsburgh
aav4@pitt.edu

MS132

Understanding Particle Diffusion in Active Suspensions: A Multiscale Study

For many micro-organisms the process of feeding results from the complex interplay between the Brownian diffusion of target particles and their transport generated by the flow field around the swimmer. Understanding particle transport in active suspensions involves considering a wide range of length scales: from the submicronic Brownian particles to the whole suspension composed of thousands if not millions of micro-swimmers. In this presentation, I will shortly introduce the tools developped during my Ph.D to simulate active suspensions at large scales (approx. 100,000 micro-swimmers), while preserving an accurate description of hydrodynamic interactions. I will also briefly present our recent developments to model Brownian suspensions. Finally, I will combine these tools to address the issue of particle transport in dilute and concentrated active suspensions. Comparisons with experimental data will be shown and the physical mechanism hidden behind the experimental results will be detailed.

Blaise Delmotte
Courant Institute
NYU
delmotte@cims.nyu.edu

MS132

Stochastic Model of Clogging in a Microfluidic Device for Sorting Flexible Cells

Microfluidic devices for sorting cells by deformability show promise for various medical purposes, e.g. detecting sickle cell anemia and circulating tumor cells. One such device is made up of sequential layers of progressively smaller channels, each layer containing identical channels in parallel. In this talk, I propose a stochastic model for the failure of microfluidic devices by clogging and present preliminary numerical results. The failure time distribution is investigated analytically in certain limiting cases.

Thomas Fai
Harvard University
tfai@seas.harvard.edu

MS132

Transition to Collective Motion and Mixing in Suspensions of Micro-Rotors

Self-organization of active objects has attracted considerable attention recently. Hydrodynamic interactions play a crucial role in the emerging behavior when the objects are immersed in fluid. While self-propelled active objects have been extensively investigated, the collective behavior of rotating active particles has received limited attention. We develop a new numerical method, based on the Immersed Boundary Framework, to trace the coupled dynamics of many rotating particles that interact with each-other and

the surrounding fluid. To elucidate the transition to collective behavior and especially the role of multi-body hydrodynamic interactions, we numerically study systems of co- and counter-rotating spheres by varying the mixture ratio as well as the total volume fraction. With increasing density, we observe the transition from chaotic behavior and small-clustering, to phase separation of rotors into macroscopic lanes or vortices.

Enkeleida Lushi
Brown University
enkeleida_lushi@brown.edu

MS133

Nonlinear Bending Theories for Intrinsically Strained Plates

This talk will present some results about critical points of the nonlinear bending energy (Willmore) functional with an isometry constraint, for plates whose reference configuration is intrinsically strained.

Peter Hornung
Technische Universität Dresden
peter.hornung@tu-dresden.de

MS133

The Intrinsic Bending and Twisting of a Rod with Misfit

A 2003 paper by Mora and Müller studied the behavior of thin elastic rods, obtaining a nonlinear bending-torsion theory as the gamma-limit of 3D elasticity. We revisit this problem, considering what happens when there is nontrivial misfit (equivalently: prestrain) which varies across the section of the rod (and perhaps along its length as well). In the thin-domain limit, what results is a rod with intrinsic bending and twist. We discuss some examples and implications, including (i) misfit as a possible explanation for why some crystals tend to twist; and (ii) connections with the existing literature on "non-Euclidean" ribbons or ribbons with surface stress.

Robert V. Kohn
Courant Institute of Mathematical Sciences
New York University
kohn@cims.nyu.edu

Ethan O'Brien
Courant Institute of Mathematical Sciences
New York University, USA
obrien@cims.nyu.edu

MS133

Plates with Incompatible Strains

We study the effective elastic behaviour of the incompatibly prestrained thin plates, characterized by a Riemann metric on the reference configuration. We prove that in the weak prestrain regime there are only two scalings possible and only two effective residual energies depending on the vanishing of appropriate Riemann tensor components.

Marta Lewicka
Department of Mathematics
University of Pittsburgh
lewicka@pitt.edu

MS133

Interpenetration of Matter in Plate Theories Obtained as Gamma-Limits

We reconsider the derivation of plate theories as Gamma-limits of 3-dimensional nonlinear elasticity and define a suitable notion for the interpenetration of matter in the limit configuration. Given a limit map satisfying this interpenetration property, we show that any recovery sequence has to consist of maps that are 2-to-1 on a set of positive measure. Then we explain how our result is applied in the context of the derivation of plate theories.

Heiner Olbermann
Hausdorff Center for Mathematics & Institute for Appl. Math.
University of Bonn
heiner.olbermann@hcm.uni-bonn.de

Eris Runa
MPI MIS Leipzig
eris.runa@mis.mpg.de

MS134

Cell-Ecm Interactions During Cancer Invasion

The extracellular matrix (ECM), a fibrous material that forms a network in a tissue, significantly affects many aspects of cellular behavior, including cell movement and proliferation. Transgenic mouse tumor studies indicate that excess collagen, a major component of ECM, enhances tumor formation and invasiveness. Moreover, cell interactions with the collagen matrix result in aligned fibers that facilitate cell invasion. However, the underlying mechanisms are unclear since the properties of ECM are complex, with diverse topographies and mechanical properties depending on various biophysical parameters. We have developed a three-dimensional elastic computational fiber network model, and parameterized it with in vitro collagen experiments. Using this model, we simulate distribution of residual stress in the gel upon local deformation, mimicking ECM remodeling from cell migration. We have also developed a 3D cell migration model that interacts mechanically with the ECM. This model is the first step toward a fully biomechanical cell-matrix interaction model for changes in matrix organization during cell migration and tumor invasion.

Yi Jiang
Georgia State University
yjiang12@gsu.edu

MS134

ChromoShake: A Chromosome Dynamics Simulator

ChromoShake is a three-dimensional simulator designed to find the thermodynamically favored states for given chromosome geometries. The simulator has been applied to a geometric model based on experimentally determined positions and fluctuations of DNA, and the distribution of cohesin and condensin in the budding yeast centromere. Simulations of chromatin in differing initial configurations reveal novel principles for understanding the structure and

function of a eukaryotic centromere.

Josh Lawrimore
Biology Department
lawrimor@email.unc.edu

Joseph Aicher, Patrick Hahn
Computer Science Dept
University of North Carolina at Chapel Hill
jkaicher@crimson.ua.edu, phahn@live.unc.edu

Alyona Fulp, Ben Kompa
Biology Department
University of North Carolina at Chapel Hill
arfulp@live.unc.edu, kompa@live.unc.edu

Leandra Vicci
Department of Computer Science
University of North Carolina
vicci@cs.unc.edu

Michael Falvo
Department of Physics and Astronomy
University of North Carolina at Chapel Hill
falvo@physics.unc.edu

Russell M. Taylor II
Department of Computer Science
University of North Carolina at Chapel Hill
taylorr@cs.unc.edu

Kerry Bloom
University of North Carolina
kerry_bloom@unc.edu

MS134

Polymeric Aspects of DNA Repair

A genome is a complete copy of the entire set of genetic material that makeup a specific organism. The genome of eukaryotes is distributed into chromosomes. Each chromosome consists of a single nucleosome fiber made up of double stranded DNA looped around histones. In addition to the challenges presented by replication, packaging and segregation, genome stability is constantly compromised by DNA damage and errors in DNA repair. Among the various forms of DNA damage, double-strand breaks (DSBs) are especially detrimental. In this talk, we combined high spatial and temporally resolved chromosome dynamics in live cells with mathematical models to elucidate the relationship between physical and biochemical properties of chromatin to process associated to the formation and repair of DSBs.

Paula A. Vasquez
University of South Carolina
paula@math.sc.edu

Kerry Bloom
University of North Carolina
kerry_bloom@unc.edu

M. Gregory Forest
University of North Carolina at Chapel Hill
Dept of Math & Biomedical Engr.
forest@unc.edu

Josh Lawrimore
Biology Department
lawrimor@email.unc.edu

MS135

Singular Limit Problem for Smectic Liquid Crystals

Abstract not available

Jinhae Park
Chungnam National University
Daejeon, South Korea
jhpark2003@gmail.com

MS135

Title Not Available

Abstract not available

Margarida M. Telo Da Gama
University of Lisbon, Portugal
mmgama@fc.ul.pt

MS135

Global Existence and Regularity of Solutions for the Active Liquid Crystal System

We consider the active hydrodynamics, described by the Q-tensor liquid crystal framework. We prove the existence of global weak solutions in dimensions two and three with suitable initial data, and obtain the higher regularity of the weak solutions and the uniqueness of weak-strong solutions in dimension two.

Gui-Qiang Chen
University of Oxford
chengq@maths.ox.ac.uk

Apala Majumdar
University of Bath
a.majumdar@bath.ac.uk

Dehua Wang
University of Pittsburgh
Department of Mathematics
dwang@math.pitt.edu

Rongfang Zhang
University of Pittsburgh
roz14@pitt.edu

MS136

On a Family of Inhomogeneous Torsional Creep Problems

The asymptotic behavior of solutions to a family of inhomogeneous PDEs in divergence form is studied in an Orlicz-Sobolev setting. Solutions are shown to converge uniformly to the distance function to the boundary of the domain. One consequence is that a well-known result in the analysis of problems modeling torsional creep continues to hold under much more general constitutive assumptions on the stress. Joint work with M. Mihăilescu (University of Craiova and "Simion Stoilow" Institute of Mathematics of the Romanian Academy, Bucharest, Romania).

Marian Bocea

Loyola University Chicago
mbocea@luc.edu

MS136

Limiting Strain Models in Elasticity Theory and Variational Integrals with Linear Growth

We investigate the properties of certain elliptic systems leading, a priori,to solutions that belong to the space of Radon measures. We show that if the problem is equipped with a so-called Uhlenbeck structure, then the solution can in fact be understood as a standard weak solution, with one proviso: analogously as in the case of minimal surface equations, the attainment of the boundary value is penalized by a measure supported on (a subset of) the boundary, which, for the problems under consideration here, is the part of the boundary where a Neumann boundary condition is imposed. Finally, we will connect such elliptic systems with certain problems in elasticity theorythe limiting strain models.

Miroslav Bulicek
Charles University
mbul8060@karlin.mff.cuni.cz

MS136

On Implicit and Strain-Limiting Theories for Describing the Elastic Response of Bodies

Abstract not available

K. R. Rajagopal
Texas A&M University
krajagopal@tamu.edu

MS136

Finitely Extensible Polymer Chains in Nematic Elastomers

In isotropic rubber elasticity there are many models of finitely extensible materials that are based on the description of a single polymer chain due to Kuhn and Grün. By generalising their arguments, a new description of a single polymer chain in a main-chain nematic elastomer as an entropic spring is obtained. The generalisation retains the finite extensibility property and couples to the entire orientation distribution function of the nematic components of the system.

Jamie M. Taylor
University of Oxford
jamie.taylor@maths.ox.ac.uk

MS137

Time-reversal Symmetry Bounds for Electromagnetic Devices

In this talk, we describe our recent work on the important consequences of time-reversal symmetry on various electromagnetic devices, stemming from fundamental bounds on the asymmetry of the electromagnetic field distribution at any point in space under excitation from different directions. In particular, we discuss how these bounds limit the performance of nonlinearity-based non-reciprocal devices, on the emission rates of a source near an asymmetric structure, and on the scattering cross-section of a 3D object versus the gain of a dipole source embedded in it. Physical insights will be discussed based on theoretical analysis and numerical simulations of realistic systems.

Andrea Au, Dimitrios Sounas
The University of Texas at Austin
alu@mail.utexas.edu, dsounas@gmail.com

MS137

Nonlinear Models of Lasers, Noise, and the Salt Equations

Abstract not available

Steven Johnson
MIT
stevenj@math.mit.edu

MS137

Lossless Polariton Solitary Waves

Session Code L;Oral presentation; No transfer to poster presentation Photons and excitons in a semiconductor microcavity interact to form exciton-polariton condensates and are governed by a nonlinear quantum-mechanical system. We calculate all non-traveling harmonic soliton solutions for the one-dimensional lossless system. There are six frequency bands, including dark, bright, and discontinuous solitons, with amplitudes ranging from 0 to infinity. The far fields of the solitons in the lowest and highest frequency bands are linearly unstable, whereas the other four bands have linearly stable far fields. With S. Komineas and S. Venakides.

Stephen P. Shipman
Department of Mathematics
Louisiana State University
shipman@math.lsu.edu

MS138

Simulating Finite-Energy Disclination Dynamics by Modeling Discontinuous Director Fields

Nonsingular disclination dynamics in a uniaxial nematic liquid crystal is modeled within a pde setting. The model alleviates the nasty singularities of classical Oseen-Frank theory related to prediction of defect equilibria. Incorporating a conservation law for the topological charge of line defects allows for the correct prediction of defect dynamics like annihilation and dissociation that would not be possible with dynamics employing just the knowledge of the energy function like an L_2 gradient flow.

Chiqun Zhang
Carnegie Mellon University
Civil and Environmental Engineering
chiqun0524@gmail.com

Xiaohan Zhang
Stanford University
xiaohanzhang.cmu@gmail.com

Amit Acharya
Civil and Environmental Engineering
Carnegie Mellon University
acharyaamit@cmu.edu

Dmitry Golovaty
The University of Akron

Department of Mathematics
dmitry@uakron.edu

Noel J. Walkington
Department of Mathematical Sciences
Carnegie Mellon University
noelw@andrew.cmu.edu

MS138

Liquid Crystal Models of Viral Capsids

The genome of virus infecting bacteria is packed in capsides often in a spooling configurations. We model a capsid as an axisymmetric eastic shell of a few nanometers in diameter. We invesigate DNA packing models based in chormonic liquid crystals and study the ensuing free boundary problems. The models account for electrostatic effects, allowing us tp estimate the effective radius of the DNA filament. The problem is motivated by experiments on bacteria-resistant antibiotics.

Javier Arsuaga
Department of Mathematics and Molecular and Cellular Biolog
University of California, Davis
jarsuaga@ucdavis.edu

MS138

Orientation of a Liquid Crystal Layer with Arbitrary Anchoring Conditions

The equilibrium orientation of a liquid crystal layer between two parallel plates with anchoring conditions either parallel or orthogonal to the plates is trivial. However, for a layer with arbitrary anchoring conditions on each plate, the orientation is much more complicated. We find a family of analytical solutions to the equilibrium Leslie-Ericksen equations for a given set of anchoring conditions and then select the solution that minimizes the free energy.

Eric P. Choate
Dept of Mathematics
University of North Carolina at Chapel Hill
echoate2@radford.edu

MS138

Electrokinetic Flows in Nematic Films with Prescribed Anchoring Patterns

In the presence of an electric field, spatial variations of the nematic director along with the anisotropy of dielectric permittivity and ions' mobilities give rise to the separation of electric charges which consequently triggers a flow of the liquid crystal. We present a model of this process and its asymptotic solutions for the flow in a nematic film with a prescribed periodic director distribution.

Oleh Tovkach
The University of Akron
otovkach@uakron.edu

MS139

The Application of the String Method to the Dislocation Dynamics

We present a numerical method to compute the transition rates including the entropy effect, of the thermally activated events in dislocation dynamics on the atomistic scale, based on the transition state theory and the string method. We also present atomistic simulation on dislocation cross-slip in aluminum, with focus on the dependence of the transition paths and energy barriers on dislocation length and position. A new mechanism with combination of the classical mechanisms has been identified.

Congming Jin
Zhejiang Sci-Tech University
jincm@lsec.cc.ac.cn

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

Weiqing Ren
National University of Singapore and IHPC, A-Star
matrw@nus.edu.sg

Gang Lu
California State University Northtridge
ganglu@csun.edu

MS139

Discrete Dislocation Dynamics with Anisotropic Elasticity Using Fast Fourier Transforms

Discrete dislocation dynamics simulations are generally limited to isotropic elasticity. Anisotropic elasticity is ignored because of the associated computational expense. We present an FFT-based formalism in which the dislocations are steps in the deformation tensor. The latter parameterizes the slip in the lattice and can be considered as an eigenstrain. The stress field arising from the dislocations is calculated with the new method, which provides the forces used to solve the equations of motion.

Anthony Rollett
Carnegie Mellon University
Materials Science and Engineering
rollett@andrew.cmu.edu

John Graham, Richard LeSar
Iowa State Univ.
jgraham@iastate.edu, lesar@iastate.edu

MS139

Homogenisation of a Row of Dislocation Dipoles

Conventional discrete-to-continuum approaches have seen their limitation in describing the collective behaviour of the multi-polar configurations of dislocations, which are widely observed in crystalline materials. The reason is that dislocation dipoles, which play an important role in determining the mechanical properties of crystals, often get smeared out when traditional homogenisation methods are applied. To address such difficulties, the collective behaviour of a row of dislocation dipoles is studied by using matched asymptotic techniques. The discrete-to-continuum transition is facilitated by introducing two field variables respectively describing the dislocation pair density potential and the dislocation pair width. It is found that the dislocation pair width evolves much faster than the pair density. Such hierarchy in evolution time scales enables us to describe the dislocation dynamics at the coarse-grained level by an evolution equation for the slowly varying variable (the pair density) coupled with an equilibrium equation for the fast varying variable (the pair width). The time-scale sepa-

ration method adopted here paves a way for properly incorporating dipole-like (zero net Burgers vector but non-vanishing) dislocation structures, known as the statistically stored dislocations (SSDs) into macroscopic models of crystal plasticity in three dimensions. Moreover, the natural transition between different equilibrium patterns found here may also shed light on understanding the emergence of the persistent slip bands (PSBs) in fatigue metals induced by cyclic loads.

Jon Chapman
Mathematical Institute
The University of Oxford
chapman@maths.ox.ac.uk

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

Yichao Zhu
Department of Mathematics
The Hong Kong University of Science and Technology
mayczhu@ust.hk

MS140

Numerical Study of Vapor Condensation and Wetting Transition on Patterned Surface Using String Method

In the first part, we study vapor condensation on hydrophobic surfaces patterned with microscale pillars. The critical nuclei, the activation barriers, and the minimum energy paths are computed using the climbing string method. In the second part, we study wetting transition on hydrophobic grooved surface using molecular dynamics. We use density field of particles as the collective variables. Then we apply climbing string method to find out the transition state in the space of collective variables.

Yunzhi Li
National University of Singapore
a0000571@u.nus.edu

MS140

A Parametric Finite Element Method for Simulating Solid-State Dewetting Problems

We propose an efficient and accurate parametric finite element method (PFEM) for solving the sharp interface model of solid-state dewetting of thin films with anisotropic surface energies. The governing equations of the sharp interface model belong to high-order geometric PDEs, which include anisotropic surface diffusion flow and contact line migration. Compared to the traditional methods, the proposed PFEM not only has good accuracy, but also poses very mild restrictions on the numerical stability.

Quan Zhao
National University of Singapore
a0109999@nus.edu.sg

MS140

A Phase Field Approach for Simulating Solid-State Dewetting of Thin Films

The capillary force drives a diffusive process in solid thin films known as dewetting. We present a phase field method to simulate dewetting and use it to study shape instabilities on solid thin films. The method is applied for a variety of geometries in two and three dimensions, and for isotropic, weakly-anisotropic, and strongly-anisotropic materials. In combination with analytical work, this method offers insights into underlying instability mechanisms and how to manipulate the final microstructure.

Rachel Zucker
University of California, Berkeley
rzucker@berkeley.edu

Rainer Backofen, Axel Voigt
TU Dresden
rainer.backofen@tu-dresden.de, axel.voigt@tu-dresden.de

W. Craig Carter
Departament of Matrials Science and Engineering
Massachusetts Institute of Technology
ccarter@mit.edu

Carl V. Thompson
Massachusetts Institute of Technology
cthomp@mit.edu

MS141

Physically Motivated Model for Creep of Microstructured Materials to Study the Composite Effects at High Temperatures

Directional solidification (DS) of NiAl-9Mo, NiAl-31Cr-3Mo, and Fe-Al leads to either a fibrous or lamellar microstructure. The DS NiAl-9Mo fibrous microstructure is highly regular, thus predestined to study the composite effects at high temperatures. A three-dimensional finite element model based on single-crystal plasticity theory for creep is introduced. The model is based on only physically motivated parameters and is evaluated with experimentally measured creep curves under several conditions. The applicability of the model to lamellar microstructures is discussed.

Jürgen Albiez
Karlsruher Institut für Technologie (KIT)
juergen.albiez@kit.edu

Ioannis Sprenger, Anke Scherf, Martin Heilmaier, Thomas Böhlke
Karlsruhe Institute of Technology
ioannis.sprenger@kit.edu, anke.scherf@kit.edu, martin.heilmaier@kit.edu, thomas.boehlke@kit.edu

MS141

Fast Numerical Calculation of Percolation and Effective Diffusivity of Random Continuum Microstructures

Strategies are presented for numerically determining the percolation threshold of two-phase random continuum microstructures. Emphasis is placed on careful sampling of the microstructures to avoid artifacts introduced by discretization. A reduction-to-the-interface method for efficiently computing the effective diffusivity of random continuum microstructures is also presented.

Thomas J. Hardin
MIT Department of Materials Science and Engineering
hardin@mit.edu

Christopher A. Schuh
MIT
Department of Materials Science and Engineering
schuh@MIT.EDU

MS141

Network Representations of Mechanical Percolation

Mechanical percolation is a phenomenon in materials processing wherein filler rod-like particles incorporated into polymeric materials enhance the composites mechanical properties. Experiments have well characterized a nonlinear phase transition from floppy to rigid behavior at a threshold filler concentration, but the underlying mechanism is not well understood. We utilize network analysis, including a rigid graph compression method, and compare with rigidity theory and spring system modeling to explore mechanical percolation.

Sam B. Heroy
UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL
SHEROY@LIVE.UNC.EDU

Dane Taylor
University of Colorado at Boulder, USA
dane.r.taylor@gmail.com

Bill Shi
UNIVERSITY OF CHICAGO
bill10@uchicago.edu

Peter J. Mucha
University of North Carolina
mucha@unc.edu

Greg Forest
UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL
forest@unc.edu

MS141

The Morphology of Lath Martensite: A New Perspective

A mathematical framework is proposed to predict the features of the (5 5 7) lath transformation in low-carbon steels based on energy minimisation. This theory generates a one-parameter family of possible habit plane normals and identifies the (5 5 7) normals as those associated with small atomic movement and maximal compatibility. While the calculations bear some resemblance to those of double shear theories, the assumptions and conclusions are different.

Anton Muehlemann
Department of Mathematics
University of Oxford
muehlemann@maths.ox.ac.uk

Konstantinos Koumatos
Gran Sasso Science Institute
konstantinos.koumatos@gssi.infn.it

MS142

Geodesic Calculus for Smooth and Discrete Shells

We present a Riemannian geodesic calculus in the space of shells based on a Riemannian metric reflecting material and physical properties of thin elastic objects. By means of this calculus one can perform operations such as shape inter- and extrapolation or statistics of shapes. As shells are discretized by triangular meshes we introduce a notion of fundamental geometric objects on triangular meshes based on concepts from discrete differential geometry to describe membrane and bending deformations.

Behrend Heeren
Rheinische Friedrich-Wilhelms-Universität Bonn
behrend.heeren@ins.uni-bonn.de

Martin Rumpf
Rheinische Friedrich-Wilhelms-Universität Bonn
Institut für Numerische Simulation
martin.rumpf@ins.uni-bonn.de

Peter Schroeder
Caltech
USA
ps@caltech.edu

Max Wardetzky
Institute of Num. and Appl. Math
University of Göttingen, Germany
wardetzky@math.uni-goettingen.de

Benedikt Wirth
Universität Münster
benedikt.wirth@uni-muenster.de

MS142

A Bending Theory for Nematic Elastomers

Nematic liquid crystal elastomers couple the elasticity of a polymer network with the anisotropy of liquid crystal molecules. The result is a solid displaying unique phenomena such as soft elasticity, spontaneous distortion and microstructure. We derive a bending type theory for thin sheets of this material via Γ-convergence assuming entropic and Frank elasticity are comparable in this regime. Many interesting features emerge from this theory, including spontaneous curvature and a design principal for active nematic glass sheets.

Paul Plucinsky
California Institute of Technology
pplucins@caltech.edu

Kaushik Bhattacharya
Howell N. Tyson Sr. Professor of Mechanics
California Institute of Technology
bhatta@caltech.edu

MS142

Elastic Curves and Surfaces in Riemannian Spaces with Applications to Interpolation of Shells

A widely-used method to interpolate points in Euclidean space is by curves that minimize their average squared sec-

ond derivative (which can be thought of as an elastic bending energy). Several formulations exist for this interpolation problem, for instance one in the framework of cubic splines, resulting in several possibilities to generalize this concept to Riemannian spaces. We present some of these approaches with applications to interpolation between multiple surfaces, interpreted as points in a Riemannian space carrying a physically motivated metric. We also present the corresponding bivariate interpolation, which compared to univariate interpolation has some additional features.

P.-A. Absil
Université catholique de Louvain
absil@inma.ucl.ac.be

Gousenbourger Pierre-Yves
Université Catholique de Louvain
pierre-yves.gousenbourger@uclouvain.be

Paul Striewski, Benedikt Wirth
Universität Münster
paul.striewski@uni-muenster.de, benedikt.wirth@uni-muenster.de

MS142

Phase Field Models with Topological Constraints

With applications in the area of biological membranes in mind, we consider the problem of minimizing Willmore's energy among the class of closed, connected surfaces with given surface area that are confined to a fixed container. Based on a phase field model for Willmore's energy due to de Giorgi, we develop a technique to incorporate the connectedness constraint into a diffuse interface model of elastic membranes. Our approach uses a geodesic distance function associated to the phase field to discern different connected components of the support of the limiting mass measure. We obtain both a suitable compactness property for finite energy sequences as well as a Gamma-convergence result. Furthermore, we present computational evidence for the effectiveness of our technique. The main argument in our proof is based on a new, natural notion of convergence to describe phase fields in three dimensions.

Stephan Wojtowytsch
Durham University
s.j.wojtowytsch@durham.ac.uk

MS143

A Three-Dimensional Elastic Model for Hydrogel Mechanics

We developed a three-dimensional bead-spring model for hydrogel using LAMMPS. We performed shear tests on the gel and found a linear relationship between the Youngs modulus and the volume fraction of gel molecule at low density. We also introduced two kinds of crosslinkers. Through simulating tensile tests, we show that increasing defects in gel structure weakens the break strength.

Hao Chen
Department of Mathematics and Statistics
Georgia State University
hchen25@student.gsu.edu

MS143

Numerical Approximation of Non-Newtonian Fluid Structure Interaction Problems

Simulating fluid-structure interactions is challenging due to the tight coupling between the solid and fluid substructures in a moving domain. Explicit and implicit decoupling methods often either fail or require relaxation when densities of the two materials are close. In this talk both monolithic and decoupling approaches are considered for the numerical study of a fluid-structure interaction problem where the fluid is governed by a viscoelastic model. A numerical algorithm which allows the problem to be stably decoupled is discussed and numerical results are presented.

Hyesuk Lee
Clemson University
Dep. of Mathematical Sciences
hklee@clemson.edu

MS143

Mathematical Insight in Biofilm Structure and Function

Bacteria are ubiquitous. Instead of living individually, bacteria appear to live in a society called a biofilm, which is a microorganism with glue-like extra-cellular polysaccharide substance. In this talk, our recent work on biofilm modeling would be presented. Special focus on the mechanism of quorum sensing and antimicrobial persistence in biofilm would be addressed, along with 3D numerical simulations. The bacteria motility issue in biofilm would be discussed, as well. Our model has been validated by our collaborators experiment results. It turns out to be an effective mathematical tool for studying biofilms.

Jia Zhao
University of South Carolina
zhaojiachina@gmail.com

MS144

Tensor Model for Bent-Core Molecules Based on Molecular Theory

Abstract not available

Jie Xu
Peking University, China
rxj_2004@126.com

MS144

Liquid-Crystalline Behavior and Elastic Properties of Homopolymer Interfaces Containing Rod-Coil Diblock Copolymers

Abstract not available

Pingwen Zhang
Peking University
pzhang@pku.edu.cn

MS144

Decoupled, Energy Stable Scheme for Continuum Hydrodynamics Allen-Cahn and Cahn-Hilliard Phase Field Model

Abstract not available

Hui Zhang

Beijing Normal University
hzhang@bnu.edu.cn

MS145

Implicit Theories for Fluids

Stokes was the first to recognize that the viscosity of many fluids varies significantly with pressure. Later, several experimental studies showed that such a variation may be exponential. The aim of this talk is to report about some basic results obtained in the framework of some theories of piezo-viscous fluids.

Giuseppe Saccomandi
Università di Perugia
giuseppe.saccomandi@unipg.it

MS145

Traveling Waves in One-Dimensional Nonlinear Models of Strain-Limiting Viscoelasticity

My talk is about traveling wave solutions of a nonlinear differential equation describing the behaviour of one-dimensional viscoelastic medium with implicit constitutive relations. I focus on a subclass of such models known as the strain-limiting models. To describe the response of viscoelastic solids a non-linear relationship among the linearized strain, the strain rate and the Cauchy stress is assumed, and traveling wave solutions corresponding to the heteroclinic connections between the two constant states is investigated. I will talk about conditions for the existence of such solutions, and then find those solutions, explicitly, implicitly or numerically, for various forms of the non-linear constitutive relation.

Yasemin Sengul
Ozyegin University, Istanbul
yasemin.sengul@ozyegin.edu.tr

MS145

On Hyperelasticity and Rank--1 Convexity for Strain--limiting Theories of Elasticity

This talk gives a brief survey of recent results concerning rank-1 convexity in the setting of implicit and strain-limiting theories of elasticity. A variety of models are considered exhibiting both isotropic and anisotropic material behavior. The theory is then applied to a consideration of the classical problem of cavitation.

Jay R. Walton
Department of Mathematics
Texas A&M
jwalton@math.tamu.edu

PP1

Some Characteristics of Resonant Transmission of a Wave Pulse

The transmitted field in a resonant transmission process consists of two distinct pathways: an initial pulse (direct transmission) and a tail of slow decay (resonant transmission). These two pathways are mathematically characterized by analyzing the poles of the scattering matrix. We analyze the effects of the coupling constant (γ), the proximity of resonance to the central frequency (η) and the spectral width (σ) of the incident pulse on resonance under the incidence of a Gaussian.

Gayan S. Abeynanda
Louisiana State University
gabeyn1@lsu.edu

Stephen P. Shipman
Department of Mathematics
Louisiana State University
shipman@math.lsu.edu

PP1

Modeling Shear Banding in Amorphous Solids Using Shear Transformation Zone Theory

The general framework of the effective temperature formalism of the shear transformation zone (STZ) theory of plasticity is tested using molecular dynamics simulation of strain localization in CuZr modeled using the embedded-atom method (EAM), amorphous Si modeled using the Stillinger-Weber (SW) potential and a binary Lennard-Jones system. Quench schedules and strain rates are varied. Effective temperature is inferred from potential energy and explored as a local coarse-grained measure of the degree of disorder.

Darius Alix-Williams
Johns Hopkins University
d.alixwill@jhu.edu

Michael L. Falk
Materials Science and Engineering
Johns Hopkins University
mfalk@jhu.edu

PP1

A Non-Affine, Conformation Tensor-Based, Viscoelastic Fluid Model

Many complex soft materials such as colloidal suspensions and blood exhibit thixotropic flow behavior. Current modeling approaches are typically phenomenological applicable only to shear flows. This work describes a new conformation tensor-based class of models, with volume constraints and two non-affine parameters, which generalizes previous emulsion/droplet-based models. Depending on the parameter values, the new model can show non-monotonic stress behavior that can lead to shear banding and/or emulate a yield stress behavior.

Antony N. Beris
University of Delaware
Newark, DE
beris@udel.edu

Paul Mwasame, Norman Wagner
University of Delaware
mwasamep@udel.edu, wagnernj@udel.edu

PP1

Three-Dimensional Simulations of Strain Localization in Metallic Glasses

We develop a three-dimensional elastoplastic simulation of a bulk metallic glass using the shear transformation zone theory. The simulations employ a recently proposed quasi-static projection method, and are run in parallel using the MPI library. By simulating metallic glasses under sim-

ple shear, we examine the nucleation and growth of shear bands in a variety of situations, paying particular attention to how they spread in the lateral direction.

Nicholas M. Boffi, Chris H. Rycroft
Harvard University
boffi@g.harvard.edu, chr@seas.harvard.edu

PP1

Thermal Fluctuations and Elastic Relaxation in the Compressed Exponential Dynamics of Colloidal Gels

We perform molecular dynamics simulation of a colloidal gel to investigate how the dynamics change with the age of the system. Upon breaking and reorganization of the network structure, the system may display stretched or compressed exponential relaxation. We show that the transition between these two regimes is associated to the interplay between thermally activated rearrangements and the elastic relaxation of internal stresses.

Mehdi Bouzid, Emanuela DelGado
Georgetown university
mb1853@georgetown.edu, emanuela.del.gado@georgetown.edu

PP1

Effect of Viscosity on Propagation of MHD Waves in Astrophysical Plasma

The study of wave dynamics in a homogeneous plasma is of fundamental interest in solar and astrophysical plasmas. Magnetohydrodynamic (MHD) instabilities play a major role in a great variety of astrophysical and space applications. We determine the general dispersion relation for the propagation of (MHD) waves in astrophysical plasma by considering the effect of gravitational instability and viscosity with anisotropic pressure tensor and heat-conducting plasma. Basic MHD equations have been derived and linearized by the method of perturbation to develop the general form of dispersion relation equation. We discussed the solutions of the dispersion relation in various special cases corresponding to the standard wave mode of stability and instability zero , low and high plasmas. Our result indicates that the transverse propagationnof waves in such a plasma is affected by the inclusion of heat conduction. For wave propagation, parallel to the magnetic field direction, we find that the fairhose mode is unaffected, whereas the mode corresponding to the gravitational instability is modified in astrophysical plasma with anisotropic pressure tensor being stable in the presence of viscosity and strong magnetic field at considerable wavelength

Alemayehu Cherkos
Kotebe University Colleg
alexye7@gmail.com

PP1

Fully Optimized Second-Order Estimates for the Macroscopic Response of Porous Viscoplastic Materials

Use is made of the recently developed fully optimized second-order homogenization method to generate estimates for the macroscopic response of power-law viscoplastic porous materials. In particular, yield surfaces will be constructed for ideally plastic matrix materials. In order to improve the results for nearly hydrostatic loading, use will also be made of an iterative variational procedure. The results will be compared with other estimates and available numerical results.

Shuvrangsu Das, Pedro Castañeda
Department of Mechanical Engineering and Applied Mechanics
University of Pennsylvania
dasshu@seas.upenn.edu, ponte@seas.upenn.edu

PP1

Defect Structures Around Two Colloidal Particles in a Nematic Liquid Crystal

Experiments show that two colloidal particles placed in a liquid crystal matrix will create defects in the surrounding medium. Our goal is to find a minimizer for the Landau-de Gennes model in order to replicate these defects numerically. The incompatibility of the liquid crystal anchoring on the container and the surface of the particle produce defects in the numerical simulations which match the observed experimental data.

Paula Dassbach
University of Minnesota
dassb004@umn.edu

PP1

Shape Minimization Problems for Structured Materials

We consider a class of problem where the configuration of a structured material must be found by minimizing the energy functional with respect to both internal fields as well as the shape of the domain, incorporating both local and global constraints. Examples include fluid-filled flexible capacitors or liquid crystal droplets with weak surface tension. We present an adaptive finite-element scheme to solve these problems and explore the effect of the physical parameters on the shape.

Andrew Debenedictis
Tufts University
andrew.debenedictis@tufts.edu

Timothy J. Atherton
Tufts University
Department of Physics
timothy.atherton@tufts.edu

PP1

Homogenization Theory for the Prediction of Obstructed Solute Diffusivity in Macromolecular Solutions

The study of diffusion in macromolecular solutions is important in many biomedical applications such as separations, drug delivery, and cell encapsulation, and key for many biological processes such as protein assembly and interstitial transport. Multiple models for the a-priori prediction of diffusion in macromolecular environments have been proposed. However, most models include parameters that are not readily measurable, are specific to the polymer-solute-solvent system, or are fitted and do not have a physical meaning. For the first time, we develop a homogenization theory framework for the prediction of effective solute diffusivity in macromolecular environments based on physical parameters that are easily measurable

and not specific to the macromolecule-solute-solvent system. Homogenization theory is useful for situations where knowledge of fine-scale parameters is used to predict bulk system behavior. As a first approximation, we focus on a model where the solute is subjected to obstructed diffusion via stationary spherical obstacles. We find that the homogenization theory results agree well with computationally more expensive Monte Carlo simulations. The homogenization theory agrees with effective diffusivities of a solute in dilute and semi-dilute polymer solutions measured using fluorescence correlation spectroscopy. Lastly, we provide a mathematical formula for the effective diffusivity in terms of a non-dimensional and easily measurable geometric system parameter.

Preston Donovan
University of Maryland, Baltimore County
pdonovan@umbc.edu

Yasaman Chehreghanianzabi
Saint Louis University
chehreghanianza@slu.edu

Muruhan Rathinam
University of Maryland, Baltimore County
muruhan@umbc.edu

Silviya Zustiak
Saint Louis University
szustiak@slu.edu

PP1

Minimizer Describing Configuration of Nematic Liquid Crystal Between Cylinders with a Core Surface Penalty

We consider a nematic liquid crystal confined between two coaxial cylinders and seek a molecular configuration which minimizes energy, assuming that the liquid crystal has planar, tangential boundary conditions on the outer cylinder. We add a term to the Oseen-Frank energy that penalizes the size of the core and show that the minimizer is either the escaped twist solution or the planar concentric solution, depending on the penalty term.

Ashley Earls, Lindsey Hiltner
University of Minnesota
earls006@umn.edu, hiltn010@umn.edu

PP1

On Some Stochastic Singular Integro-Partial Differential Equations and the Parabolic Transform

Some stochastic singular integro-partial differential equations are studied without any restrictions on the characteristic forms of the partial differential operators. Linear and nonlinear cases are studied. Using the parabolic transform, existence and stability results are obtained. The Cauchy problem of fractional stochastic partial differential equations can be considered as a special case from the obtained results. Key words: Singular integral equations, Stochastic partial differential equations, Existence and stability of solutions, Fractional stochastic partial differential equations.

Mahmoud M. El-Borai
Prof.of Math. Dep. of Mathematics Faculty of Science Alexandria University Alexandria Egypt
m_m_elborai@yahoo.com

Khairia E. El-Nadi
Prof of Mathematical Statistics Dep. of Math. Faculty of Science Alexandria University Alexandria Egypt
Khairia_el_said@Hotmail.com

PP1

A Mechano-Hydraulic Model of Intracranial Pressure Dynamics

Monitoring the intracranial pressure of the brain provides clinicians with valuable physiological information for patients in critical condition. In the following paper, we will present a new mechano-hydraulic mathematical model that allows one to study the dynamics arising from the coupling between the mechanics of brain, CSF circulation, and cerebral blood flow. We will examine the dynamics of the model and perform a bifurcation analysis to examine domains of stability.

Davis Evans
The Pennsylvania State University
Department of Engineering Science and Mechanics
dje5104@psu.edu

Corina Drapaca
Department of Engineering Science and Mechanics
Pennsylvania State University
csd12@psu.edu

Joseph Cusumano
The Pennsylvania State University
Department of Engineering Science and Mechanics
jpc3@psu.edu

PP1

Phase-Field Modeling of Alloy Solidification Using Quaternions and Calphad Input

An implicit time-stepping finite volume algorithm for the simulation of microstructure evolution during the solidification of an alloy is presented. The approach is based on a phase-field model including a phase variable, a quaternion orientation variable, and the alloy composition. Energies and diffusion coefficients are based on thermodynamic and kinetic databases in the framework of the CALPHAD methodology. Numerical results for solidification in alloys of interest to additive manufacturing are used to illustrate the methodology. Prepared by LLNL under Contract DE-AC52-07NA27344

Jean-Luc Fattebert
Lawrence Livermore National Lab.
fattebert1@llnl.gov

PP1

Nucleation and Growth of Cavities in Gels

Many body implantable devices are made of synthetic polymer which upon insertion absorb water, causing the polymer to swell and forming a gel (mixture of solid and fluid). Since the swelling leads to an expansion of the polymer, a gel is considered as a compressible material. A high concentration of stress due to the swelling leads to the nucleation and growth of cavities within the gel, likely to cause the debonding of the material from a support it is attached to. In this research, we focus on the cavitation in a gel occupying a spherical domain, applying a uniform extensional stress at the boundary of the domain. We consider a to-

tal energy of the gel which accounts for the compressible elasticity of the polymer and the mixing between polymer and fluid, called Flory-Huggins energy. In addition to penalizing gel deformation, the energy presents competing effects of entropy that favours mixing, polymer-polymer and fluid-fluid interaction forces. We study material properties necessary to allow for a nucleation, characterization of radially symmetric deformations and stability analysis of the cavity.

Robert Foldes, Maria-Carme Calderer
University of Minnesota
fold0023@umn.edu, calde014@umn.edu

PP1

Second-Order Homogenization Estimates for the Yield Domain of Composite Materials

This poster deals with the determination of the homogenized yield domain of rigid-ideally plastic composites. For this purpose, variational estimates that are exact to second-order in the contrast are generated for the homogenized dissipation functions of the plastic composites, in terms of the homogenized dissipation functions of fully optimized linear comparison composites. Sample results are given and compared with earlier bounds for the effective yield domain of two-phase isotropic composites, as well as fiber-reinforced composites.

Joshua Furer
Department of Applied Mathematics and Computational Science
University of Pennsylvania
jfurer@sas.upenn.edu

Pedro Ponte-Castañeda
Department of Mechanical Engineering and Applied Mechanics
University of Pennsylvania
ponte@seas.upenn.edu

PP1

Discontinuous Galerkin Methods For Modeling Reactive Interfaces in Photoelectrochemical Solar Cells

The dynamics of charge transport within photoelectrochemical solar cells are described by systems of drift-diffusion-Poisson equations. The stiffness of each system and the reactive coupling across the semiconductor-electrolyte interface greatly complicate numerical simulations. We will discuss numerical algorithms, mainly based on local discontinuous Galerkin methods, domain decomposition methods, and implicit-explicit time stepping techniques, that were developed specifically to overcome these obstacles. Results on algorithm performance and simulations of nanostructured solar cells will be presented.

Michael D. Harmon
Institute for Computational and Engineering Sciences
mharmon@ices.utexas.edu

PP1

Using Correlation Coefficient for Determining Suitability of Eddy Current Testing for Quality Control of Heat Treated Steel

Non-destructive eddy current testing (ET) method has been employed for characterization of 51CrV4 steel. Different micro-structures have been obtained by heat treatment of samples at different temperatures and time. ET signature of each sample has been obtained in the form of permeability and impedance and correlation coefficient (R2) was established. The technique has been effectively applied to differentiate and isolate non-conforming heat treated parts during mass production. High correlation coefficients (R2) were acquired for different heat treatments and corresponding ET response.

Javeria Hashmi
National University of Science and technology (NUST)
National University of Sciences and Technology Islamabad
hashmi001@ymail.com

PP1

Modeling Viral DNA Packing in a 2D Circular Domain

The packing of DNA into a viral capsid must be very efficient; the DNA strand is much longer than the capsid, is negatively charged, and is very stiff. Due to the highly confined environment, the packing can be modeled as a continuum, and one can use the theories of nonlinear elasticity and liquid crystals to do so. We consider a two-dimensional circular capsid and analyze parameter values of the model, making comparisons to experimental data.

Lindsey Hiltner
University of Minnesota
hiltn010@umn.edu

PP1

Deformation in Metallic Glass: Connecting Atoms to Continua

Metallic glasses like other amorphous solids experience strain localization as the primary mode of failure. However, the development of continuum constitutive laws which provide a quantitative description of disorder and mechanical deformation remains an open challenge. Recent progress has shown the necessity of accurately capturing fluctuations in material structure, in particular the statistical changes in potential energy of the atomic constituents during the non-equilibrium process of applied shear. Here we directly cross-compare molecular dynamics shear simulations of a ZrCu glass with continuum shear transformation zone (STZ) theory representations. We present preliminary results for a methodology to coarse-grain detailed molecular dynamics data with the goal of initializing a continuum representation in the STZ theory.

Adam R. Hinkle
Johns Hopkins University
ah353@cornell.edu

PP1

An Autogenous Friction Stir Spot Welding Rig for Modelling Heat Generation in Friction Stir Processing

Modelling of friction stir processing depends critically on knowledge of: (a) the constitutive response of the alloy as a function of temperature and strain-rate; (b) the flow and thermal fields in the thermomechanically affected zone. A new experimental rig has been developed for validation of constitutive data and heat generation using autogenous friction stir spot welding, and tested for a range of Al and

Mg alloys. The experiments are modelled using Lagrangian and Eulerian numerical methods.

Patryk Jedrasiak
Harvard University
patryk.jedrasiak@gmail.com

Hugh Shercliff
University of Cambridge
hs10000@cam.ac.uk

Chris H. Rycroft
Harvard University
chr@seas.harvard.edu

PP1

Hybrid Reduced Basis Method and Generalized Polynomial Chaos for Stochastic Partial Differential Equations

The generalized Polynomial Chaos(gPC) method is a popular method for solving partial differential equations (PDEs) with random parameters. However, when the probability space has high dimensionality, the solution ensemble size required for an accurate gPC approximation can be large. Therefore, it may incur excessive computational burden. We show that this process can be made more efficient by closely hybridizing gPC with Reduced Basis Method (RBM). Since the reduced model is more efficient, costs are significantly reduced. We demonstrate that this is achieved with essentially no loss of accuracy through numerical experiments.

Jiahua Jiang
University of Massachusetts, Dartmouth
jjiang@umassd.edu

PP1

Stability of Multiscale/multiphysics Simulation of Laser Propagation in Optically-Active Semiconductors

We discuss the numerical stability of calculations of the interaction between a laser light field and the non-linear polarization of an optically-active semiconductor medium (GaN). This coupling strongly influences the laser propagation. We have adapted the streamline-upwind/Petrov-Galerkin finite element method (FEM) to compute the laser propagation within the paraxial approximation. We compute the medium polarization local to the FEM Gauss points, coupling medium-light-field response using sequential multi-scale/multi-physics coupling, with explicit Euler time stepping.

Brent Kraczek
US Army Research Laboratory
brent.e.kraczek.civ@mail.mil

Jaroslaw Knap
U.S. Army Research Laboratory
jaroslaw.knap.civ@mail.mil

PP1

VoroTop: Voronoi Cell Topology Visualization and Analysis Toolkit

This poster describes VoroTop, a modern set of open-source tools for analyzing structure of spatial point sets in three dimensions, using a complete description of the Voronoi cell topology of each point. VoroTop provides robust, structure-independent tools that can characterize and identify structure in ordered and disordered systems. One particular strength is its ability to visualize defects in highly-perturbed crystals, at temperatures close to melting.

Emanuel A. Lazar
University of Pennsylvania
Department of Materials Science and Engineering
mlazar@seas.upenn.edu

Jian Han, David J. Srolovitz
University of Pennsylvania
jianhan@seas.upenn.edu, srol@seas.upenn.edu

PP1

A Computational Framework for Scale Bridging in Multiscale Simulations

We have developed an adaptive computational framework for multiscale modeling that allows for rapid construction of multiscale models through composition of individual at-scale models. The framework incorporates scalable numerical algorithms including: i) adaptive computational strategies, ii) algorithms for scale-bridging, and iii) algorithms for development of surrogate models. We will describe our computational framework and highlight its use in developing a multiscale model of an energetic material and a high-throughput capability for battery research.

Kenneth Leiter, Jaroslaw Knap, Brian Barnes, Richard Becker, Oleg Borodin
U.S. Army Research Laboratory
kenneth.w.leiter2.civ@mail.mil,
jaroslaw.knap.civ@mail.mil,
brian.c.barnes11.ctr@mail.mil,
richard.c.becker.civ@mail.mil,
oleg.a.borodin.civ@mail.mil

PP1

Brittle to Ductile Transition in a Model of Sheared Granular Materials

Understanding physics of deformation and failure in Granular materials is crucial for many natural phenomena and industrial processes Here we present a computational 2D in-plane strain model for large deformation viscoplasticity in sheared granular materials based on the shear transformation zone theory. We explore possible brittle to ductile transition in granular rheology as a function of initial porosity, grain size, and strain rate. We discuss implications of this transition for earthquake rupture dynamics.

Xiao Ma
University of Illinois at Urbana-Champain
xiaoma5@illinois.edu

Ahmed Elbanna
Department of Civil and Environmental Engineering
University of Illinois, Urbana-Champaign
elbanna2@illinois.edu

PP1

Direct Structure-Property Relations Mining in Scanning Tunneling Microscopy: Markov Random

Field and Convolutional Neural Network Approach

We present a novel method for positional and rotational information extraction from individual molecules imaged at nanometer length scale by scanning tunneling microscopy. We utilize Markov Random Field (MRF) model for polar rotational state decoding and combined convolutional Neural Network and MRF model for azimuthal rotational state identification. We demonstrate the effectiveness of the approach by utilizing it on buckybowl self-assembled monolayer to identify the presence of rotational domains and non-trivial boundary structure.

Artem Maksov
Bredesen Center, University of Tennessee Knoxville
Oak Ridge National Laboratory
amaksov@vols.utk.edu

Maxim Ziatdinov
Oak Ridge National Laboratory
ziatdinovma@ornl.gov

Shintaro Fujii, Manabu Kiguchi
Tokyo Institute of Technology
fujii.s.af@m.titech.ac.jp, kiguti@chem.titech.ac.jp

Shuhei Higashibayashi
Institute for Molecular Science
higashi@ims.ac.jp

Hidehiro Sakurai
Osaka University
hsakurai@osaka-u.ac.jp

Sergei Kalinin
Oak Ridge National Laboratory
sergei2@ornl.gov

Bobby Sumpter
ORNL
sumpterbg@ornl.gov

PP1

Flow of a Drilling Fluid Between Two Rotating Cylinders

We study the fully developed Couette flow of a drilling fluid, and explore the effects of concentration and shear-rate-dependent viscosity. The one-dimensional form of the governing equations, as well as the boundary conditions are made dimensionless and a parametric study is performed by varying the dimensionless numbers.

Mehrdad Massoudi
National Energy Technology Laboratory
U. S. Department of Energy
MASSOUDI@NETL.DOE.GOV

Weitao Wu
Wei-Tao Wu ¡weitaow@andrew.cmu.edu¿
Carnegie Mellon University
weitaow@andrew.cmu.edu

PP1

Resonant Electromagnetic Scattering in Layered Media with Random Fabrication Errors

The delicate resonance phenomena in slab structures that support electromagnetic guided modes are of particular interest in the manufacture of optical devices such as light-emitting diodes. A guided mode appears as an eigenvalue embedded in the continuous spectrum of the underlying Maxwell operator. Perturbing the system elicits anomalous scattering behavior near the guided mode frequency, called Fano resonance. We quantify the sensitivity of this resonance to random perturbations of the material coefficients of the slab.

Emily A. Mchenry
Louisiana State University
Department of Mathematics
emchen2@lsu.edu

PP1

Parameter Identification for Creep Modeling in Polymers for Accurate Manufacture

Accurate manufacture with micrometer accuracy is a difficult task to achieve in polymer parts because of their unstable structure at room temperature. Any measurement with a contact probe which lasts continuously for minutes or hours can cause creep deformation in a polymer specimen. In the present work a numerical creep model is proposed and in this context the needed material parameters are obtained by two different approaches: (i) nonlinear regression and (ii) smoothing of the experimental data and extraction of the derivatives from logarithmic transformations. These two methods are compared with experimental results and it is found that the smoothing approach is the general and suited for the purpose. Since it is not dependent on an initial guess as is the nonlinear regression.

Ali Mohammadi
Technical University of Denmark
Anker Engelunds Vej 1 Bygning 101A 2800 Kgs. Lyngby
almoha@mek.dtu.dk

Mads Rostgaard Sonne, Giuseppe Dalla Costa, Daniel Gonzalez-Madruga, Leonardo De Chiffre, Jesper Henri Hattel
Technical University of Denmark
mrso@mek.dtu.dk, giucos@mek.dtu.dk, dagoma@mek.dtu.dk, ldch@mek.dtu.dk, jhat@mek.dtu.dk

PP1

Topology Optimization of Hyperelastic Continua

Topology optimization (TO) has various potential applications in early phases of structural design. However, most research on TO has focused on linear elastic materials, which has severely restricted applications of TO to hyperelastic structures made of, e.g., rubber or elastomer. The contribution of this research is an investigation of different models of hyperelastic materials and their influences on the resulting topologies, which are demonstrated by numerical examples including a simple tire model.

Trung Pham, Christopher Hoyle, Yue Zhang
Oregon State University
phamtr@oregonstate.edu, chris.hoyle@oregonstate.edu, zhangyue@oregonstate.edu

Tam H. Nguyen
Surbana Jurong Private Limited
Singapore

nguyenhongtam@gmail.com

PP1

General Theory of Spontaneous Emission Near Exceptional Points

While it is well known that resonant cavities can enhance spontaneous emission rates, recent work suggests that giant enhancements can occur when two resonances coalesce into an exceptional point (EP). In fact, traditional expressions for the enhancement formally diverge at EPs. We develop a general theory of emission at EPs, which uses Jordan-vector perturbation theory, and we show that the enhancement is actually finite and depends critically on the amount of gain in the system.

Adi Pick
Harvard University
adipick@physics.harvard.edu

Bo Zhen
Massachusetts Institute of Technology
bozhen@mit.edu

Owen D. Miller
Math Dept.
Massachusetts institute of Technology
odmiller@math.mit.edu

Chia Hsu
Yale University
chiawei.hsu@yale.edu

Felipe Hernandez
Massachusetts Institute of Technology
felipeh@mit.edu

Alejandro Rodriguez
Princeton University
arod@princeton.edu

Marin Soljacic
Massachusetts Institute of Technology
soljacic@mit.edu

Steven Johnson
MIT
stevenj@math.mit.edu

PP1

Kinetics of the Triple Line in Solid-state Wetting

We analyze the kinetics of the triple-line of thin solid films during spreading or dewetting. We show that the departure from equilibrium at the triple line can be related to the kinetics at the micro or meso-scopic level. A continuum model is designed to describe triple in non-equilibrium situations. This model is related to non-equilibrium triple line kinetics via an asymptotic analysis. We discuss the influence of these findings on growth or dewetting dynamics.

Olivier Pierre-Louis
Université J. Fourier Grenoble 1
olivier.pierre-louis@univ-lyon1.fr

Ashwani Tripathi
Univ. C. Bernard Lyon 1
ashwani.jnu@gmail.com

PP1

Coarse-Graining in Metallic Glasses from Molecular Dynamics to Continua

Metallic glasses, like other amorphous materials, present complexities in their mechanical properties due to their disordered structure - making it hard to predict their failure, specifically through the formation of shear bands. Current theories postulate there exists a critical length-scale over which plastic deformation can be characterized via shear-transformation zones (STZs) defined by the structure of the material, specifically the density of STZs. The effective disorder temperature formalism, as an indirect measure of STZ density, is connected with the average atomic potential energy in molecular dynamics (MD) simulations. In this way, the results from MD simulations assist the study of plastic deformation in the continuum STZ theory. We perform the coarse-graining of the MD atomic potential energies for Cu64Zr36 metallic glasses using a Gaussian windowing function whose standard deviation establishes the critical length-scale for disorder temperature characterization. The coarse-graining length-scale is therefore independent of the resolution for the continuum simulation input, which can be refined to the necessary degree for numerical convergence. By investigating different coarse-graining length-scales, those corresponding to the characteristic length-scale for disorder temperature have been established, and the noise inherent in the MD data has been effectively reduced for the purpose of the continuum study.

Dihui Ruan
The Johns Hopkins University
druan1@jhu.edu

Adam R. Hinkle, Michael D. Shields
Johns Hopkins University
ah353@cornell.edu, michael.shields@jhu.edu

Chris H. Rycroft
Harvard University
chr@seas.harvard.edu

Michael L. Falk
Materials Science and Engineering
Johns Hopkins University
mfalk@jhu.edu

PP1

Discrete Systems with Degenerated Growth

We consider lattice systems with random interactions between the lattice points. We assume that the interaction potentials satisfy growth conditions which are degenerated and are given in terms of certain weight functions. We show that under suitable integrability assumptions for the weight functions and stationarity/ergodicity assumptions for the interaction potentials the discrete energy Γ-converges almost surely to a deterministic and homogenous integral functional.

Mathias Schäffner
University of Würzburg (Germany)
mathias.schaeffner@tu-dresden.de

Stefan Neukamm
Technische Universität Dresden

Institute for Scientific Computing
stefan.neukamm@tu-dresden.de

Anja Schlömerkemper
University of Würzburg
anja.schloemerkemper@mathematik.uni-wuerzburg.de

PP1

Approximate Global Minimizers to Pairwise Interaction Problems

We present a new analytic based approach for finding approximate global minimizers to pairwise interaction problems. The approach relies on a convex relaxation of the primal pairwise interaction problem that allows for a straightforward solution using standard optimization techniques. Moreover, we show how one can use the solution to the relaxed problem to generate approximate minimizers with recovery guarantees. The advantage of the approach is that it may predict non-standard patterns, and in some cases may be exact. The approach also generates a dual decomposition for the interaction energy that leads to the emergence of length scales preferred by low energy structures.

David Shirokoff
New Jersey Institute of Technology
david.g.shirokoff@njit.edu

PP1

Homogenized Response of Porous Plastic Single Crystals

Rigorous bounds on the macroscopic plastic behavior of nonlinear porous single crystals are computed by means of a recently developed iterated variational linear comparison homogenization method. In particular, Hashin-Shtrikman bounds in the form of gauge (yield) surfaces are reported for porous cubic and hexagonal single crystals with varying degrees of porosity, nonlinearity and crystal anisotropy.

Dawei Song, Pedro Ponte Castañeda
University of Pennsylvania
songdaw@seas.upenn.edu, ponte@seas.upenn.edu

PP1

Microscale FEA Homogenization Procedure for Use in Elastography Inversions

A finite element model of an axonal (white matter) structure is presented to enable higher fidelity non-linear inversion (NLI) methodologies for magnetic resonance elastography (MRE). A computational homogenization method is developed, allowing for determination of the effective properties of a complex representative volume element (RVE). Sensitivity analysis and optimization procedures are performed to enable integration of a microscale RVE into a macroscale procedure for use within existing imaging modalities.

Assimina A. Pelegri, Daniel Sullivan
Rutgers - The State University of New Jersey
pelegri@jove.rutgers.edu, danielsu@rutgers.edu

PP1

Phase Delay for a b-Function Model of Viscoelastic Behaviour

Empirically, resin composites under steady loading relax according to: $\Psi(t;b,\tau) = exp[-(t/\tau)^b]; b < 0,5$. In fatigue testing, this anelasticity causes a time delay δt between load and measured displacement. Expressing $\Psi(t;b,\tau)$ as a sum of exponential decays, scaled by $\tau_n = \tau \cdot 10^{n/4b}$, the weighting is virtually independent of b. The Laplace transformation relating δt to τ and b is derived and applied.

John E. Tibballs
NIOM, Nordic Institute for Dental Materials
jot@niom.no

PP1

Local Rearrangements of Droplets in a Dense Emulsion Under Shear

Rheology of jammed emulsions, simultaneously performing confocal microscopy, is presented in this work. In addition to experiments, we perform molecular dynamics simulations of repulsive soft spheres, which complement the experimental observations and provide a detailed picture of microscopic rearrangement of jammed droplets under shear deformation. Measuring the shear-frame Mean Square Displacement, displacement distributions, non-Gaussian parameter and displacement correlations we show the distinct differences in droplet rearrangement approaching the the dynamical yield stress.

Vishwas Venkatesh, Sudeep Dutta, Emanuela Del Gado, Daniel Blair
Georgetown University
vv120@georgetown.edu, skd623@yahoo.com, ed610@georgetown.edu, dlb76@georgetown.edu

PP1

Computing Links Between Effective Tensors of Pairs of Fiber-Reinforced Elastic Composites with the Same Microstructure

In certain special cases, called "links' it is possible to express the effective tensor of a composite material in terms of the effective tensor of another composite, whose microstructure is the same as the first, but the material properties of the constituents are different. General theory of links defines them as a superposition of several complicated transformations. The goal of my research was to represent each link in a mathematically beautiful form.

Patrick M. Wynne, Hansen Pei, Abe Lyle
Temple University
patrick@temple.edu, tuf28625@temple.edu, tuf21034@temple.edu

PP1

Multiscale Material Model Development for Accident Tolerant Fuels: Bottom-Up

Use of uraniumsilicide (U-Si) is one of the promising concepts being to increase the accident tolerance of nuclear fuels. In this talk, we will present our recent progress on multiscale material model development for accident tolerant fuels, spanning density functional theory calculations, molecular dynamics potential development, phase field simulation and engineering scale modeling. Our ultimate goal is to develop knowledge-based models for use at the macro-

scopic scale with a minimum of empirical parameters.

Jianguo Yu, Jason Hales, Yongfeng Zhang
Idaho National Laboratory
Jianguo.Yu@inl.gov, jason.hales@inl.gov, yongfeng.zhang@inl.gov

PP1

On the Mathematical Structure of the Laws Governing the Fundamental Forces of Nature: A New Axiomatic Matrix Approach

In this article I present a new axiomatic matrix approach based on the ring theory and the generalized Clifford algebra. On the basis of this approach, by linearization (and simultaneous parameterization), followed by first quantization of the relativistic energy-momentum relation (for a particle), a unique set of the general relativistic (single-particle) wave equations are derived directly. These equations are shown to correspond to the massive forms of equations of motion of the fundamental fields, including the laws governing the fundamental forces, i.e. the gravitational, electromagnetic and nuclear field equations (only for 4D spacetime), and the (half-integer spin) particle wave equations such as Dirac equation (only for 3D space-time). In particular, the massive form of the general theory of relativity - with a definite complex torsion - is obtained by first quantization of a special relativistic relation. In addition, the (local) gauge invariance of Lagrangian for the obtained massive form of Yang-Mills fields has been proven where these fields formally are re-presented on a curved background spacetime with a complex torsion. Based on the equations derived and assuming the parity symmetry (for free particle fields), I've shown that the universe cannot have more than four spacetime dimensions. Moreover, an argument for the asymmetry of left and right handed (interacting) particles is presented. (http://adsabs.harvard.edu/abs/2015arXiv150101373Z)

Ramin Zahedi
Hokkaido University
zahedi@let.hokudai.ac.jp

PP1

Toward a Variantional Principle of Space Charge Stimulated Discharge in Electron Irradiated PMMA

Electron-irradiated materials have been widely used. Space-charge distribution due to irradiated electrons may cause electrical breakdown in materials producing fractal patterns. Fractal-growth based models have been developed to generate similar patterns. We, however, analyze the dynamics from a new perspective. We find a relationship between ionization and a modified electrical conduction law, which corresponds to the solution of an optimization problem. Thus a mechanism by which the local process of ionization acts to globally optimize a fractal discharge channel is formulated.

Xuewei Zhang
Texas A&M University - Kingsville
ZHANGXW2012@GMAIL.COM

PP1

Transformation Groups and Discrete Structures in Continuum Description of Defective Crystals

Davinis description of a defective crystal involves 3 continuum 'lattice vector' fields, interpreted as averages, and a scalar dislocation density matrix. Those fields are to describe the kinematics of a defective crystal, and may allow for elastic and plastic deformations in particular. A constitutive assumption, namely that the functional dependence of energy on dislocation density can be truncated to derivatives up to a certain order, leads us to consider finite dimensional algebras of 'lattice vector' fields and corresponding transformation groups. In low spatial dimensions, such groups may be classified. We discuss discrete structures which emerge in this context as discrete subgroups of corresponding Lie groups. Such structures includes the usual crystal lattices as a particular case.

Maxim Zyskin
Department of Math.,University of Bristol
maxim.zyskin@nottingham.ac.uk