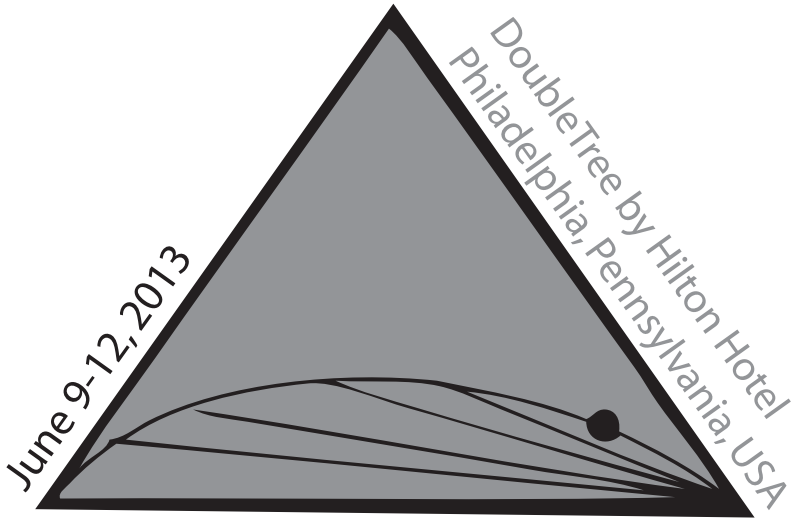
Final Program and Abstracts



SIAM Conference on

Mathematical Aspects of Materials Science

Sponsored by the SIAM Activity Group on Mathematical Aspects of Materials Science

The purpose of the SIAM Activity Group on Mathematical Aspects of Materials Science (SIAG/MS) is to bring together mathematicians, engineers and scientists interested in the application of analysis and computation to problems in materials science. The SIAG serves as a meeting point for mathematicians, engineers and scientists from all areas of computational and materials science, thus fostering cross-fertilization between fields, and from diverse venues such as academia, industry and the national laboratories.

2013 is designated as the year of Math of Planet Earth.
SIAM supports MPE2013.
http://www.crm.umontreal.ca/Math2013/en/

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Max Planck Institute for Mathematics in the Sciences, Germany

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SIAM Registration Desk

The SIAM registration desk is located in Overture. It is open during the following times:

Saturday, June 8
4:00 PM - 8:00 PM

Sunday, June 9
7:00 AM - 5:30 PM

Monday, June 10
7:30 AM - 5:30 PM

Tuesday, June 11
7:30 AM - 5:30 PM

Wednesday, June 12
7:30 AM - 5:30 PM

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List current April 2013.

Funding Agencies

SIAM and the conference organizing committee wish to extend their thanks and appreciation to the U.S. National Science Foundation and the U.S. Department of Energy for their support of this conference.

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All other concurrent/breakout rooms will have one (1) screen and one (1) data projector. Cables or adaptors for Apple computers are not supplied, as they vary for each model. Please bring your own cable/adaptor if using a Mac computer. Overhead projectors will be provided only when requested.

If you have questions regarding availability of equipment in the meeting room of your presentation, or to request an overhead projector for your session, please see a SIAM staff member at the registration desk.

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Email stations are available to attendees during registration hours.

SIAM attendees booked within the SIAM room block will have complimentary wireless Internet access in their guest rooms. Complimentary wireless Internet access in the hotel lobby and Standing O Restaurant will also be available. Wireless email access is available in the conference meeting space to all participants.

Registration Fee Includes

- Admission to all technical sessions
- Business Meeting (open to SIAG/MS members)
- Coffee breaks daily
- Room set-ups and audio/visual equipment
- Poster Session
- Welcome Reception

Job Postings

Please check with the SIAM registration desk regarding the availability of job postings or visit *http://jobs.siam.org*.

Important Notice to Poster Presenters

The poster session is scheduled for Sunday, June 9 at 9:00 PM. Poster presenters are requested to set up their poster material on the provided 4' x 8' poster boards in the Orchestra no later than 8:00 PM, the official start time of the Poster Spotlight Session. Boards and push pins will be available to presenters beginning Sunday, June 9 at 12:00 PM. Posters will remain on display through 10:15 AM on Wednesday, June 12. Poster presenters be sure to remove your poster by 10:15 AM on Wednesday, June 12. Posters remaining after this time will be discarded. SIAM is not responsible for discarded posters.

SIAM Books and Journals

Display copies of books and complimentary copies of journals are available on site. SIAM books are available at a discounted price during the conference. If a SIAM books representative is not available, completed order forms and payment (credit cards are preferred) may be taken to the SIAM registration desk. The books table will close at 1:30 PM on Wednesday, June 12.

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A space for emergency contact information is provided on the back of your name badge. Help us help you in the event of an emergency!

Comments?

Comments about SIAM meetings are encouraged! Please send to:

Sven Leyffer, SIAM Vice President for Programs (*vpp@siam.org*)

Get-togethers

- **Welcome Reception**
  Saturday, June 8
  6:00 PM – 8:00 PM

- **Poster Session**
  Sunday, June 9
  9:00 PM – 11:00 PM

- **Business Meeting**
  (open to SIAG/MS members)
  Tuesday, June 11
  8:15 PM – 9:00 PM
  Complimentary beer and wine will be served.

Please Note

SIAM is not responsible for the safety and security of attendees' computers. Do not leave your laptop computers unattended. Please remember to turn off your cell phones, pagers, etc. during sessions.

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Audio and video recording of presentations at SIAM meetings is prohibited without the written permission of the presenter and SIAM.

Social Media

SIAM is promoting the use of social media, such as Facebook and Twitter, in order to enhance scientific discussion at its meetings and enable attendees to connect with each other prior to, during and after conferences. If you are tweeting about a conference, please use the designated hashtag to enable other attendees to keep up with the Twitter conversation and to allow better archiving of our conference discussions. The hashtag for this meeting is #SIAMMS13.

SIAM Activity Group on Mathematical Aspects of Materials Science (SIAG/MS)

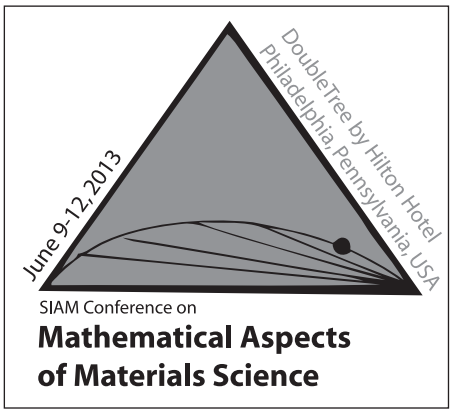
www.siam.org/activity/materials_science

A GREAT WAY TO GET INVOLVED!

Collaborate and interact with mathematicians and applied scientists whose work involves mathematical aspects of materials science.

ACTIVITIES INCLUDE:

- Special sessions at SIAM Annual Meetings
- Biennial Conference
- Wiki



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- Listing in the SIAG's online membership directory
- Additional $10 discount on registration for the SIAM Conference on Mathematical Aspects of Materials Science (excludes student)
- Electronic communications about recent developments in your specialty
- Eligibility for candidacy for SIAG/MS office
- Participation in the selection of SIAG/MS officers

ELIGIBILITY:

- Be a current SIAM member.

COST:

- $10 per year
- Student members can join two activity groups for free!

2009—2010 SIAG/MS OFFICERS:

- Chair: Maria-Carme Calderer, University of Minnesota
- Vice Chair: Robert Lipton, Louisiana State University
- Program Director: Felix Otto, Max Planck Institute for Mathematics in the Sciences
- Secretary: Dio Margetis, University of Maryland College Park

TO JOIN:

SIAG/MS: my.siam.org/forms/join_siag.htm
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Invited Plenary Speakers

*** All Invited Plenary Presentations will take place in Symphony - 3rd Floor****

Sunday, June 9

8:15 AM – 9:00 AM

IP1 Motility at Microscopic Scales

Antonio De Simone, *SISSA, Italy*

9:00 AM – 9:45 AM

IP2 Wrinkle Patterns in Thin Sheets

Benny Davidovitch, *University of Massachusetts, Amherst, USA*

1:30 PM – 2:15 PM

IP3 Asymptotics-based Model Reduction in Electronic Structure: Old and New

Gero Friesecke, *Technische Universität München, Germany*

Monday, June 10

8:15 AM – 9:00 AM

IP4 Scaling in Kinetic Mean-field Models for Coarsening Phenomena

Barbara Niethammer, *University of Bonn, Germany*

9:00 AM – 9:45 AM

IP5 Numerical Methods in Molecular Dynamics

Tony Lelievre, *CERMICS ENPC, France*

1:30 PM – 2:15 PM

IP6 Tracking Multiphase Physics: Geometry, Foams, and Thin Films

James Sethian, *University of California, Berkeley, USA*

Invited Plenary Speakers

Tuesday, June 11

8:15 AM – 9:00 AM

IP7 Toward the Principles of Self Assembly and Self Replication

Michael Brenner, *Harvard University, USA*

9:00 AM – 9:45 AM

IP8 Organic Crystal Growth in Thin Films

Anette Hosoi, *Massachusetts Institute of Technology, USA*

1:30 PM – 2:15 PM

IP9 Metamaterials: High Contrast Composites with Unusual Properties

Graeme W. Milton, *University of Utah, USA*

Wednesday, June 12

8:15 AM – 9:00 AM

IP10 The Dynamics of Liquid Crystals

Peter Palffy-Muhoray, *Kent State University, USA*

9:00 AM – 9:45 AM

IP11 Multiscale Mathematics and Renewable Energy

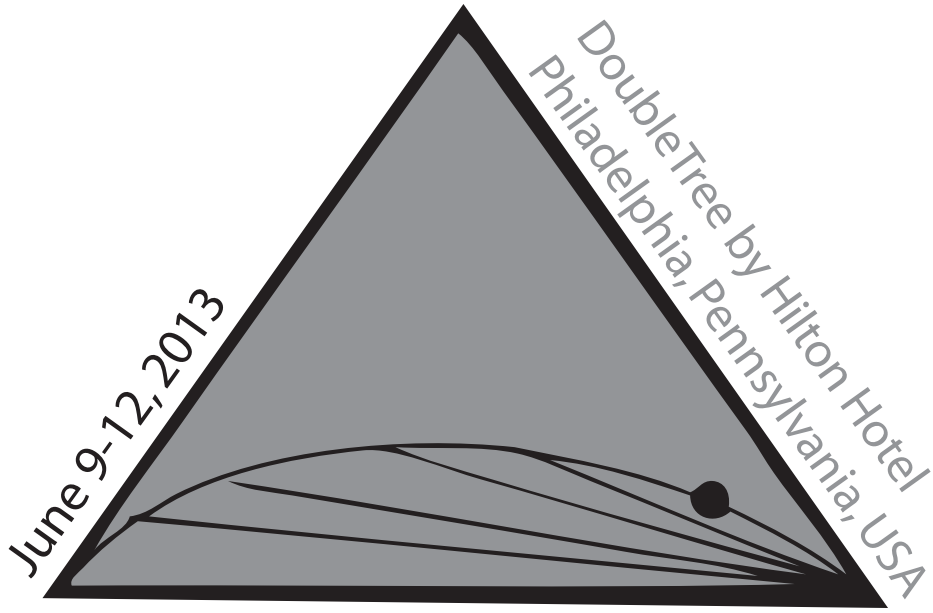
Steven Hammond, *National Renewable Energy Laboratory, USA*

1:30 PM – 2:15 PM

IP12 How Do Crystals Melt?

Weinan E, *Princeton University, USA*

Program and Abstracts



SIAM Conference on

Mathematical Aspects of Materials Science

Saturday, June 8

Registration
4:00 PM-8:00 PM

Room:Overture - 3rd Floor

Welcome Reception
6:00 PM-8:00 PM

Room:Balcony - 2nd Floor

Sunday, June 9

Registration
7:00 AM-5:30 PM

Room:Overture - 3rd Floor

Welcome Remarks
8:00 AM-8:15 AM

Room:Symphony - 3rd Floor

IP1
Motility at Microscopic Scales
8:15 AM-9:00 AM

Room:Symphony - 3rd Floor

Chair: John Ball, University of Oxford, United Kingdom

Motility of cells is at the root of many fundamental processes in biology: from sperm cells swimming to fertilize an egg cell, to metastatic tumor cells crawling to invade nearby tissues. We will discuss the mechanical bases of cellular motility by swimming and crawling. Special emphasis will be placed on the connections between low Reynolds number swimming and Geometric Control Theory, and on the geometric structure of the underlying equations of motion. As a concrete example, we will report on reverse engineering of the euglenoid movement. The lessons learned in the context of swimming motility will be then applied to selected case studies of crawling motility.

Antonio De Simone
SISSA, Italy

IP2
Wrinkle Patterns in Thin Sheets
9:00 AM-9:45 AM

Room:Symphony - 3rd Floor

Chair: Robert V. Kohn, Courant Institute of Mathematical Sciences, New York University, USA

When confined in space, solid sheets exhibit a variety of patterns, often described as folds, blisters, wrinkles, creases, and crumples. The most elementary deformation type emerges from the classical buckling-wrinkling instability of thin objects under compressive loads. Nevertheless, experiments on nano-metrically thin sheets have shown that standard "post-buckling" theory fails to predict basic features of wrinkle patterns. I will describe some recent developments in studies of wrinkling phenomena, emphasizing the "far-from-threshold" theory, a singular perturbation approach to address wrinkles in very thin, highly-bendable sheets. Focusing on class of "simplest yet nontrivial" (radial stretching) models that exhibits the morphological complexity of thin sheets, I will describe the principles of the FFT wrinkling theory, and a few mechanisms by which wrinkles give way to other patterns.

Benny Davidovitch
University of Massachusetts, Amherst, USA

Coffee Break
9:45 AM-10:15 AM

Room:Assembly - 3rd Floor

Sunday, June 9

MS1

Stochastic Homogenization: Quantitative Theory and Application to Materials Science - Part I of II

10:15 AM-12:15 PM

Room:Symphony - 3rd Floor

For Part 2 see MS46

Homogenization theory for PDEs with random coefficients can been used to characterize the bulk properties of a material having random microstructural properties. These two sessions explore recent theoretical and computational advances in homogenization theory for stochastic equations. In particular, they focus on a quantitative version of the theory (including fluctuation and error estimation), on efficient numerical computation tools, and on novel applications to materials.

Organizer: Antoine Gloria
Université Libre de Bruxelles, Belgium

Organizer: James Nolen
Duke University, USA

10:15-10:40 Normal Approximation for Random Elliptic Equations
James Nolen, Duke University, USA

10:45-11:10 Quantitative Homogenization of the Heat Equation with Random Coefficients
Jean-Christophe Mourrat, École Polytechnique Fédérale de Lausanne, Switzerland

11:15-11:40 Homogenization of Elliptic Pde in Random Environments with Long--range Correlations
Joseph Conlon, University of Michigan, USA

11:45-12:10 Limit Theorems for the Random Conductance Model
Marek Biskup, University of California, Los Angeles, USA

Sunday, June 9

MS2

Multiscale Modeling, Microstructure, and Local Field Properties of Heterogeneous Media - Part I of III

10:15 AM-12:15 PM

Room:Aria B - 3rd Floor

For Part 2 see MS20

The special session is aimed at presenting recent developments concerning the "micro-macro" interconnection in heterogeneous materials. The session will bring together experts that will focus on the recent developments and current challenges in the homogenization of partial differential equations with oscillatory coefficients, fine-scale stress concentration modeling, nonlocal continuum modeling, peridynamics, complexity reduction and multiscale computational modeling with applications to composites, suspensions, and biomaterials.

Organizer: Lyudmyla Barannyk
University of Idaho, USA

Organizer: Yuliya Gorb
University of Houston, USA

Organizer: Silvia Jimenez
Worcester Polytechnic Institute, USA

10:15-10:40 Kinetic Equation for Spatial Averages of Particle Dynamics
Alexander Panchenko, Washington State University, USA

10:45-11:10 Time-averaging of ODE Systems with Highly Oscillatory Response
Amit Acharya, Carnegie Mellon University, USA; Marshall Slemrod, University of Wisconsin, Madison, USA; Likun Tan, Carnegie Mellon University, USA

11:15-11:40 Statistical Mechanical Foundation of the Peridynamic Nonlocal Continuum Theory
Rich Lehoucq, Sandia National Laboratories, USA

11:45-12:10 Statistical Foundations of Liquid-Crystal Theory
Brian Seguin and Eliot Fried, McGill University, Canada

Sunday, June 9

MS3

Multiscale Computation of Fluctuating Hydrodynamics and Microscale Mechanics - Part I of III

10:15 AM-12:15 PM

Room:Aria A - 3rd Floor

For Part 2 see MS30

The hydrodynamics of complex fluids, such as polymer solutions, colloidal suspensions and reactive fluid mixtures, has recently attracted great interest. Coarse-grained models cover a broad range of time and length scales by incrementally sacrificing physical fidelity for computational efficiency. This minisymposium will focus on advances in multiscale numerical methods for simulating flows and biomechanical structures at mesoscopic scales. Issues to be discussed will cover the inclusion of thermal fluctuations in analytical and computational models, coupling of continuum fluids to immersed structures and calibration of effective parameters.

Organizer: Christel Hohenegger
University of Utah, USA

Organizer: Scott McKinley
University of Florida, USA

Organizer: Aleksandar Donev
Courant Institute of Mathematical Sciences, New York University, USA

10:15-10:40 Coupling a Fluctuating Fluid to Immersed Particles
Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA; Florencio Balboa Usabiaga, Universidad Autonoma de Madrid, Spain; Boyce Griffith, New York University, USA; Rafael Delgado-Buscalioni, Universidad Autonoma de Madrid, Spain

10:45-11:10 Fluctuation-Dissipation Based Integrators for Brownian Dynamics
Nawaf Bou-Rabee, Rutgers University, Camden, USA

continued on next page

Sunday, June 9

MS3

Multiscale Computation of Fluctuating Hydrodynamics and Microscale Mechanics - Part I of III

continued

11:15-11:40 Immersed Particle Dynamics in Flucuating Fluids with Memory
Christel Hohenegger, University of Utah, USA; Scott McKinley, University of Florida, USA

11:45-12:10 Modeling of Thermal Fluctuations in Multicomponent Reacting Systems
Alejandro Garcia, San Jose State University, USA; John B. Bell and Kaushik Balakrishnan, Lawrence Berkeley National Laboratory, USA; Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA

Sunday, June 9

MS4

Metric-driven Deformation of Thin Elastic Sheets - Part I of III

10:15 AM-12:15 PM

Room:Concerto A - 3rd Floor

For Part 2 see MS31

The shape of a thin sheet in R^3 relects its preference for isometric embedding, and its resistance to bending. When the sheet is Euclidean, isometric embeddings are developable surfaces. But non-Euclidean sheets occur in nature (due to differential growth) and can also be created in the laboratory. We are just beginning to understand how the sheet's metric and its mechanical properties conspire to determine the shape it assumes in space. This 3-part minisymposium highlights the area's interdisciplinary character, combining geometry with analysis, physics with mathematics, and experiment with theory.

Organizer: Robert V. Kohn
Courant Institute of Mathematical Sciences, New York University, USA

10:15-10:40 How Bilayer Shape Influences Bilayer Bending
Silas Alben, University of Michigan, USA; Bavani Balakrisnan and Elisabeth Smela, University of Maryland, USA

10:45-11:10 Elastic Theory for Shape Selection of Self-Assembled Macromolecular Ribbons
Hillel Aharoni, The Hebrew University of Jerusalem, Israel; Eran Sharon, The Hebrew University, Israel

11:15-11:40 Blister Patterns and Energy Minimization in Compressed Thin Films on Compliant Substrates
Jacob Bedrossian, Courant Institute of Mathematical Sciences, New York University, USA

11:45-12:10 Shape Transitions in Hyperbolic Non-Euclidean Plates
John A. Gemmer and Shankar C. Venkataramani, University of Arizona, USA

Sunday, June 9

MS5

Micro-to-Macro Coarse-Graining and Effective Dynamics in Nonequilibrium Systems - Part I of III

10:15 AM-12:15 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS32

This symposium will bring together speakers who work on Nonequilibrium problems related to materials at various lengthscales ranging from atomic to polycrystalline.

Organizer: Kaushik Dayal
Carnegie Mellon University, USA

10:15-10:40 From Simple Particle Models to Thermodynamic Flows
Johannes Zimmer, University of Bath, United Kingdom

10:45-11:10 Unexpected Thermodynamic Properties of Some Exact Far-from-equilibrium Solutions in Molecular Dynamics
Richard James, University of Minnesota, USA

11:15-11:40 Multi-Time Scale Modeling of Dynamics of Phase Transition
Likun Tan, Amit Acharya, and Kaushik Dayal, Carnegie Mellon University, USA

11:45-12:10 Effective Dynamics of Phase Transitions in Nonlocal Fokker-Planck Equations
Michael Herrmann, Saarland University, Germany; Barbara Niethammer and Juan Velazquez, University of Bonn, Germany

Sunday, June 9

MS6

Recent Developments in Modeling Crystallization and Material Properties with Periodic Fields - Part I of III

10:15 AM-12:15 PM

Room:Rhapsody - 4th Floor

For Part 2 see MS33

Employing free energy functionals that are minimized by periodic fields allows one to study a variety of phenomena including nucleation and growth, epitaxial growth, yield strength of polycrystals, grain boundary melting and glass formation. This approach is the basis of dynamical classical density functional theory and phase field crystal models. There has been tremendous activity in this field including applications in liquid crystals, ordering on curved surfaces and hydrodynamic/ crystal interaction. This minisymposium will explore recent advances in three major avenues namely specific applications in material science, extensions to more complex systems and the connection between various approaches and traditional methods.

Organizer: Arvind Baskaran
University of California, Irvine, USA

Organizer: Ken Elder
Oakland University, USA

Organizer: John Lowengrub
University of California, Irvine, USA

10:15-10:40 Kinetic Density Functional Theory - Time Dependent Hydrodynamic Density Functional Theory for Freezing
Arvind Baskaran, University of California, Irvine, USA; Aparna Baskaran, Brandeis University, USA; John Lowengrub, University of California, Irvine, USA

continued in next column

10:45-11:10 Density Functional Theory and Phase-Field-Crystal Modelling for Liquid Crystalline and Active Systems
Hartmut Lowen, Heinrich-Heine Universitaet Duesseldorf, Germany

11:15-11:40 Scale Coupling in Phase-Field-Crystal Modeling of Materials Growth
Zhi-Feng Huang, Wayne State University, USA

11:45-12:10 Solidification Fronts in Supercooled Liquids: How Rapid Fronts Can Lead to Disordered Glassy Solids
Andrew Archer and Uwe Thiele, Loughborough University, United Kingdom; Edgar Knobloch, University of California, Berkeley, USA

Sunday, June 9

MS7

The Ginzburg-Landau Model and Related Topics - Part I of V

10:15 AM-12:15 PM

Room:Minuet - 4th Floor

For Part 2 see MS34

The focus of the minisymposium is on mathematical problems related to Ginzburg-Landau model with application in physics and materials science including but not limited to: superconductivity, superfluidity, liquid crystals, and polymers. The speakers in this minisymposium will describe their recent research including the development and structure of singular solutions of the Ginzburg-Landau-type problems and the dynamics of vortex motion.

Organizer: Yaniv Almog
Louisiana State University, USA

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Leonid Berlyand
Pennsylvania State University, USA

10:15-10:40 The Superheating Current for a Reduced Ginzburg-Landau Model
Yaniv Almog, Louisiana State University, USA

10:45-11:10 Kinematic Vortices in a Thin Film Driven by An Electric Current
Lydia Peres Hari and Jacob Rubinstein, Technion Israel Institute of Technology, Israel; *Peter Sternberg*, Indiana University, USA

11:15-11:40 Thin Film Superconductors in Strong Magnetic Fields
Stan Alama, *Lia Bronsard*, and Bernardo Galvao-Sousa, McMaster University, Canada

11:45-12:10 Vortices for a Two-Component Ginzburg-Landau Model
Stan Alama and Qi Gao, McMaster University, Canada

Sunday, June 9

MS8

Electronic Structure - Part I of IV

10:15 AM-12:15 PM

Room:Maestro A - 4th Floor

For Part 2 see MS35

Predicting the elctronic structure of complex molecular and condensed-matter systems has been a focus of attention in chemistry and physics for decades. More recently, espceically since the advent of density functional theory (DFT), it has also become an important ingredient in materials science. Electronic structure models allows the on-the-fly computation of non-empirical and chemically specific interatomic interactions within larger-scale simulations.

Organizer: Gero Friesecke
Technische Universität München, Germany

Organizer: Eric Cances
Ecole des Ponts and INRIA, France

Organizer: Lin Lin
Lawrence Berkeley National Laboratory, USA

Organizer: Chao Yang
Lawrence Berkeley National Laboratory, USA

10:15-10:40 Semiclassical Approximations to Electronic Structure via Density/Potential Functionals
Kieron Burke and Raphael Ribeiro, University of California, Irvine, USA

10:45-11:10 Numerical Analysis of Augmented Plane Wave Methods for Full-Potential Electronic Structure Calculations
Huajie Chen, Technische Universität München, Germany

11:15-11:40 BerkeleyGW: A Massively Parallel Tool for Computing Quasiparticle and Optical-Properties of Materials
Jack Deslippe, National Energy Research Scientific Computing Center, USA

11:45-12:10 Strong Correlation in Density Functional Theory
Paola Gori-Giorgi, Vrije Universiteit Amsterdam, The Netherlands

Sunday, June 9

MS9

Mathematical Crystallography: Geometric Foundations - Part I of III

10:15 AM-12:15 PM

Room:Maestro B - 4th Floor

For Part 2 see MS36

Geometric Crystallography forms a major part of the foundations of "Mathematical Crystallography, and has an ancient association with the theory of polyhedra and polytopes. It played a role in the development of abstract group theory and it relies on the theory of manifolds. The demand for new mathematical tools for crystallography entails a demand for the geometry that underlies them.

Organizer: Gregory McColm
University of South Florida, USA

Organizer: Massimo Nespolo
Université de Lorraine, France

10:15-10:40 Minimal Interface Structures
Frank Morgan, Williams College, USA

10:45-11:10 Polyhedral Geometries and Symmetry
Egon Schulte, Northeastern University, USA

11:15-11:40 Nanostructures Arising from Crystallographic Tilings
Ma. Louise N. de las Penas, Ateneo de Manila University, Philippines

11:45-12:10 Capturing the Essence of Infinite Graphs in Quotient Graphs
Bernd Souvignier, Radboud University, The Netherlands

Lunch Break

12:15 PM-1:30 PM

Attendees on their own

Sunday, June 9

IP3

Asymptotics-based Model Reduction in Electronic Structure: Old and New

1:30 PM-2:15 PM

Room:Symphony - 3rd Floor

Chair: Richard James, University of Minnesota, USA

It has long been recognized that asymptotic analysis of well chosen scaling limits is a useful alternative (or companion) to semi-empirical methods in the design of reduced electronic structure models. Due to the curse of dimensionality of the full N-electron Schrödinger equation, reduced models are necessary to facilitate the computation of ab-initio energy levels or potential energy surfaces for large systems. Early examples which have retained importance to this day include Dirac's (1930) and Becke's (1988) exchange energy functionals. In the talk I will focus on 1) asymptotics-based wavefunction methods which capture the anomalous filling order of transition metal atoms, missed e.g. by density functional theory (DFT) even with the best known functionals such as B3LYP. (Theory: G.F., B.Goddard, SIAM J. Math. Anal. 41, 2009; application to transition metals: Ch.Mendl, G.F., J.Chem.Phys.133, 184101, 2010). 2) exchange-correlation functionals in DFT emerging from the semiclassical limit of the (exact but unwieldy) Hohenberg-Kohn functional. The study of this limit was initiated by Seidl, Perdew, Levy, Gori-Giorgi and Savin, and leads, perhaps unexpectedly, into optimal transportation theory (C.Cotar, G.F., C.Klüppelberg, Comm. Pure Appl. Math. 66, 548-599, 2013).

Gero Friesecke
Technische Universität München, Germany

Intermission

2:15 PM-2:30 PM

Sunday, June 9

MS10

Homogenization and Applications - Part I of III

2:30 PM-4:30 PM

Room:Symphony - 3rd Floor

For Part 2 see MS37

This minisymposium proposal is concerned with recent developments in homogenization and its applications for modeling and understanding the overall response of various types of heterogeneous material systems. The specific topics include nonlinear constitutive behaviors, including finite elasticity and plasticity, as well as coupled properties, including applications to elasto-plastic behavior, ferroelectric and thermoelectric composites, and shape memory polycrystals. In addition, the MS includes presentations dealing with recent advances on universal bounds, instabilities for nematic liquid crystal elastomers, atomistic-to-continuum multi-scale modeling and phononic transport. The 12 presentations are organized in 3 sessions as follows (presenters are shown in boldface).

Organizer: Pedro Ponte Castaneda
University of Pennsylvania, USA

Organizer: Pierre M. Suquet
CNRS, France

2:30-2:55 Homogenization and Plasticity: Variational Approximations
Pierre M. Suquet, CNRS, France

3:00-3:25 An Energy-Based Variational Approach to Incremental Homogenization of Elasto-Visco-Plastic Composites
Laurence Brassart, Université Catholique de Louvain, Belgium; *Laurent Stainier*, Ecole Centrale de Nantes, Université de Nantes, CNRS, France; Issam Doghri and Laurent Delannay, Université Catholique de Louvain, Belgium

continued in next column

3:30-3:55 Homogenization and Elastoplasticity
Gilles Francfort, Université de Paris Nord, France

4:00-4:25 The Nonlinear Elastic Response of Suspensions of Rigid Inclusions in Rubber
Oscar Lopez-Pamies and Taha Goudarzi, University of Illinois at Urbana-Champaign, USA; Kostas Danas, Ecole Polytechnique, France

Sunday, June 9

MS11

Methods and Applications in the Optimization of Materials Composition - Part I of II

2:30 PM-4:30 PM

Room:Aria B - 3rd Floor

For Part 2 see MS74

The fundamental variables in materials design are the materials' compositions. Due to the essentially infinite space of possible materials, it is necessary to develop efficient methods for optimizing properties of materials. Compositional materials design is a mixed discrete and continuous optimization problem since each composition may support several stable arrangements of its constituent elements leading to complex and high-dimensional surfaces. Current development efforts run from deterministic branch-and-bound or (local) gradient-based methods to (global) stochastic algorithms, with and without constraints. The symposium will cover recent advances in the development and application of optimization algorithms to the materials design problem.

Organizer: Berend C. Rinderspacher
Army Research Laboratory, USA

2:30-2:55 First Principles View on Chemical Compound Space
O. Anatole von Lilienfeld, Argonne National Laboratory, USA

3:00-3:25 The Harvard Clean Energy Project: Finding Renewable Energy Materials One Screensaver at a Time
Alan Aspuru-Guzik, Harvard University, USA

3:30-3:55 Algorithms for Discovery of Nanoporous Materials for Energy Applications
Richard Martin and Maciej Haranczyk, Lawrence Berkeley National Laboratory, USA

4:00-4:25 Data Mined Compound and Crystal Structure Prediction for High-Throughput Materials Discovery
Geoffroy Hautier, Université Catholique de Louvain, Belgium

Sunday, June 9

MS12

Complex Fluids: Modeling and Simulation - Part I of II

2:30 PM-4:30 PM

Room:Aria A - 3rd Floor

For Part 2 see MS48

Complex fluids are materials with a complicated microstructure, materials that can exhibit both viscous and elastic behavior, for example polymer and colloidal solutions. Properties of these fluids can be exploited to produce materials useful in industrial (soaps and gels) and biological (blood flow and drug delivery) applications. The physics and dynamics of complex fluids are nontrivial, requiring detailed modeling combined with intricate analytic and simulation methods. The goal of this symposium is to bring together mathematicians and practitioners in the area to advance the subject through discussion and collaboration.

Organizer: Michael Cromer
University of Delaware, USA

Organizer: Lin Zhou
New York City College of Technology, USA

2:30-2:55 Modeling and Simulation of Shear Banding in Polymer Solutions from a Monotonic Constitutive Curve
Michael Cromer, University of Delaware, USA; Glenn Fredrickson and Gary Leal, University of California, Santa Barbara, USA

3:00-3:25 Diffusive Effects on the Transient and Steady State Shear Response of the Vcm Model
Lin Zhou, New York City College of Technology, USA; Pam Cook, University of Delaware, USA; Gareth H. McKinley, Massachusetts Institute of Technology, USA

3:30-3:55 Modeling and Simulation of Shear Banding Phenomena in Concentrated Solutions of Wormlike Micelles
Natalie Germann, L. Pamela Cook, Antony N. Beris, and Norman J. Wagner, University of Delaware, USA

continued in next column

4:00-4:25 Mesoscale Modeling and Simulation of Transient Networks
Yun Zeng and L. Pamela Cook, University of Delaware, USA; Lin Zhou, New York City College of Technology, USA; Gareth H. McKinley, Massachusetts Institute of Technology, USA

Sunday, June 9

MS13

Stress-induced Wrinkling of Thin Elastic Sheets - Part I of II

2:30 PM-4:30 PM

Room:Concerto A - 3rd Floor

For Part 2 see MS49

The wrinkling or folding of thin sheets is familiar - examples include the coarsening of folds in a hanging drape; the wrinkling of a sheet wrapping a piece of fruit; and the buckling of a compressed thin film. The variety of patterns is great, and we are just beginning to understand how to analyze, simulate, and harness them. This two-part minisymposium highlights the area's interdisciplinary character, combining mathematics with mechanics, experiment with theory, and analysis with computing.

Organizer: Peter Bella
Max Planck Institute for Mathematics in the Sciences, Germany

2:30-2:55 Wrinkling of a Stretched Annular Elastic Thin Sheet - Identification of the Optimal Scaling Law for the Energy of a Ground State
Peter Bella and Felix Otto, Max Planck Institute for Mathematics in the Sciences, Germany

3:00-3:25 Instabilities in Axisymmetrically Constrained Sheets
Jose Bico, École Supérieure de Physique et de Chimie Industrielles, France; Benoit Roman, PMMH-ESPCI, France; Jeremy Hure, LCMMI-CEA, France; Miguel Pineirua, ENSTA ParisTech, France

3:30-3:55 Wrinkling Behavior of Highly Stretched Rectangular Elastic Films via Parametric Global Bifurcation
Tim Healey, Cornell University, USA

4:00-4:25 Stretch-induced Wrinkling of Thin Sheets: Experiments and Modeling
Vishal Nayyar, K. Ravi-Chandar, and *Rui Huang*, University of Texas at Austin, USA

Sunday, June 9

MS14

Computational Tools for Metastable Systems - Part I of III

2:30 PM-4:30 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS41

Many materials, including crystals, metals and biological media, possess metastable states that introduce a severe time scale separation. Consequently, direct numerical simulations may be unable to observe important transitions, such as the migration of a defect through a crystal or the folding of a protein. A variety of techniques have been proposed to accelerate these computations, including accelerated dynamics and kinetic Monte Carlo. In this minisymposium, we present recent advances and analysis of such techniques.

Organizer: Gideon Simpson
University of Minnesota, USA

Organizer: Jonathan Weare
University of Chicago, USA

Organizer: Arthur F. Voter
Los Alamos National Laboratory, USA

Organizer: Mitchell Luskin
University of Minnesota, USA

2:30-2:55 Combining Hyperdynamics with the Quasicontinuum Method
Arthur F. Voter, Los Alamos National Laboratory, USA; Woo Kyun Kim and Mitchell Luskin, University of Minnesota, USA; Danny Perez, Los Alamos National Laboratory, USA; Ellad B. Tadmor, University of Minnesota, USA

3:00-3:25 A Scalable Method to Compute Transition Rate Prefactors
Danny Perez, Chen Huang, and Arthur F. Voter, Los Alamos National Laboratory, USA

3:30-3:55 A Mathematical Analysis of Temperature Accelerated Dynamics
David Aristoff, University of Minnesota, USA

4:00-4:25 A Posteriori Estimates for Accelerated Dynamics
Gideon Simpson, University of Minnesota, USA

Sunday, June 9

MS15

Parsing Experimental and Simulation Data: Pattern Extraction, Analysis, and Reproduction - Part I of II

2:30 PM-4:30 PM

Room:Rhapsody - 4th Floor

For Part 2 see MS42

New simulation and data acquisition techniques in materials science provide us with large amounts of raw data that represent materials on scales ranging from the mesoscopic to the atomistic. Consequently, the issues of how to: (1) extract and represent the mesoscopic material structure, (2) understand and represent this structure in terms of appropriate statistical descriptors, and (3) generate new raw data which is faithful to such statistical descriptors in order to perform further numerical studies must be addressed in order to allow for model validation or the analysis of material behavior. The minisymposium discusses mathematical methods related to these issues.

Organizer: Benedikt K. Wirth
Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Matt Elsey
Courant Institute of Mathematical Sciences, New York University, USA

2:30-2:55 Triple Junctions in Microstructure Design
Oliver Johnson and *Christopher A. Schuh*, Massachusetts Institute of Technology, USA

3:00-3:25 Evaluating Microstructural Parameters of Three-dimensional Grains Generated by Phase-field Simulation or Other Voxel-based Techniques
Kunok Chang, Katholieke Universiteit Leuven, Belgium

continued in next column

3:30-3:55 Grain Topologies in Three Dimensional Polycrystalline Microstructures
Emanuel A. Lazar, Columbia University, USA; Jeremy K. Mason, Lawrence Livermore National Laboratory, USA; Robert D. MacPherson, Institute for Advanced Study, USA; David J. Srolovitz, University of Pennsylvania, USA

4:00-4:25 Statistical Analyses of Complex Microstructures and Its Application to Coarsening Phenomena
Chal Park, University of Michigan, USA; Peter W. Voorhees, Northwestern University, USA; *Katsuyo Thornton*, University of Michigan, USA

Sunday, June 9

MS16

Mathematical Advances in Liquid Crystals - Part I of II

2:30 PM-4:30 PM

Room:Minuet - 4th Floor

For Part 2 see MS43

Liquid crystals are a state of matter intermediate between an isotropic liquid and a crystalline solid in that they are uniquely characterized by orientational order and possibly some positional order. They are widely used in the display industry and are good candidates for other applications such as optical metamaterials, actuators and sensors. The aim of this minisymposium is to gather scientists from around the world to discuss modeling, analysis, and simulations of liquid crystalline materials as well as related experimental results. Among other issues, the speakers will describe their recent work in liquid crystal suspensions, hydrodynamics, materials forming quasicrystals, etc.

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Xiaoyu Zheng
Kent State University, USA

2:30-2:55 Cryo-Tem Imaging of Thermotropic Bent-Core Liquid Crystals
Antal Jakli and Cuiyu Zhang, Kent State University, USA

3:00-3:25 Orientation Waves: The Order Parameter for Some QuasiCrystals
Rolfe Petschek and Brian M. Cox, Case Western Reserve University, USA; Amir Haji -Akbari, Princeton University, USA; Sharon Glozer and Michael Engel, University of Michigan, USA

3:30-3:55 Topological Defects and the Ground State Manifold
Randall Kamien, University of Pennsylvania, USA

4:00-4:25 Analysis of An Active Liquid Crystal Suspension Model
Qi Wang, University of South Carolina, USA

Sunday, June 9

MS17

Mathematical Aspects of Singularity Formation in Thin Liquid Flows - Part I of II

2:30 PM-4:30 PM

Room:Maestro A - 4th Floor

For Part 2 see MS44

Liquid films of micro- or nanoscale thickness occur widely in nature and industrial processes such as e.g. printing, spraying and electrowetting. Their qualitative behavior differs substantially from the behavior on larger scales since the interplay between surface tension and other intermolecular interactions becomes important. Rupture or coalescence of thin films as well as motion of contact lines typically lead to the formation of singularities in the pressure or liquid profile. The minisymposium provides a platform to investigate these singularities from an analytical, numerical and modeling perspective.

Organizer: Hans Knuepfer
University of Bonn, Germany

Organizer: Georgy Kitavtsev
Max Planck Institute for Mathematics in the Sciences, Germany

2:30-2:55 Towards a Regularity Theory for Thin-film Equations
Lorenzo Giacomelli, University of Rome La Sapienza, Italy

3:00-3:25 Singularities in Electrified Liquid Drops and Jets
Marco A. Fontelos, Institute for Mathematics, CSIC, Spain

3:30-3:55 On the Moving Contact Line Singularity in Diffuse-Interface Approaches
David N. Sibley and Andreas Nold, Imperial College of London, United Kingdom; Nikos Savva, Cardiff University, United Kingdom; Serafim Kalliadasis, Imperial College London, United Kingdom

4:00-4:25 Evolution of Clean Foams
Stephen H. Davis, Northwestern University, USA

Sunday, June 9

MS18

Nonlinear Lattice Dynamics - Part I of III

2:30 PM-4:30 PM

Room:Maestro B - 4th Floor

For Part 2 see MS45

Many problems in materials science concern phenomena where an interplay between discreteness and dynamics plays a fundamental role. Examples include propagation of defects, pattern formation and emergence of complexity and the application range from metamaterials to granular media. The main mathematical issues concern interaction between nonlinearity and dispersion, extremely ragged energy landscapes, trapping, depinning and radiative damping. This minisymposium features talks by leading experts in nonlinear lattice dynamics and aims at facilitating the exchange of ideas and at highlighting the most important unsolved problems in this field.

Organizer: Anna Vainchtein
University of Pittsburgh, USA

Organizer: Lev Truskinovsky
Ecole Polytechnique, France

2:30-2:55 Grain Boundaries and Dislocations in the Swift-Hohenberg Equation
Arnd Scheel, University of Minnesota, Minneapolis, USA

3:00-3:25 Defects and Ripples in Graphene
Luis Bonilla, Universidad Carlos III de Madrid, Spain; Ana Carpio, Universidad de Complutense de Madrid, Spain

3:30-3:55 Force-extension Curves of Biomolecules
Ana Carpio, Universidad Complutense de Madrid, Spain; Luis Bonilla, Universidad Carlos III de Madrid, Spain; Antonio Prados, Universidad de Sevilla, Spain

4:00-4:25 Compatibility Conditions and Damage Spread in Lattices
Andrej V. Cherkaev, University of Utah, USA

Sunday, June 9

Coffee Break

4:30 PM-5:00 PM

Room:Assembly - 3rd Floor

MS19

Aspects of Homogenization: Analysis and Applications - Part I of II

5:00 PM-7:00 PM

Room:Symphony - 3rd Floor

For Part 2 see MS28

In the last few decades, numerous studies have focused on the relationship between microscopic descriptions of large systems and the overall effective (e.g., elastic, thermal, electrical) parameters that govern the system macroscopic behavior. Applications range from models of dislocation dynamics in solids to the design of optimal high-performance composites and metamaterials to the characterization of effective properties of biological and biophysical systems. With this minisymposium, we aim to bring together experts in homogenization who work on diverse problems related to Materials Science and Biophysics. A goal is to identify emergent approaches and discuss results that shed light on properties of complex systems.

Organizer: Dionisios Margetis
University of Maryland, College Park, USA

Organizer: Antoine Mellet
University of Maryland, USA

5:00-5:25 Effective Properties of Bacterial Suspensions
Leonid Berlyand, Pennsylvania State University, USA; Igor Aranson, Northwestern University and Argonne National Laboratory, USA; Brian Haines, Los Alamos National Laboratory and Pennsylvania State University, USA; Dmitry Karpeev, Argonne National Laboratory, USA; Shawn Ryan, ; Falko Ziebert, University of Freiburg, Germany

continued in next column

5:30-5:55 Polyharmonic Homogenization, Rough Polyharmonic Splines and Sparse Super-localization
Houman Owhadi, California Institute of Technology, USA; Lei Zhang, Shanghai Jiao Tong University, China; Leonid Berlyand, Pennsylvania State University, USA

6:00-6:25 Random Fluctuations Beyond the Homogenization Limit
Guillaume Bal, Columbia University, USA

6:30-6:55 Homogenization of Dislocation Dynamics
Nicolas Forcadel, CEREMADE Universite Paris 9 Dauphine, France

Sunday, June 9

MS20

Multiscale Modeling, Microstructure, and Local Field Properties of Heterogeneous Media - Part II of III

5:00 PM-7:00 PM

Room:Aria B - 3rd Floor

For Part 1 see MS2
For Part 3 see MS47

The special session is aimed at presenting recent developments concerning the "micro-macro" interconnection in heterogeneous materials. The session will bring together experts that will focus on the recent developments and current challenges in the homogenization of partial differential equations with oscillatory coefficients, fine-scale stress concentration modeling, nonlocal continuum modeling, peridynamics, complexity reduction and multiscale computational modeling with applications to composites, suspensions, and biomaterials.

Organizer: Lyudmyla Barannyk
University of Idaho, USA

Organizer: Yuliya Gorb
University of Houston, USA

Organizer: Silvia Jimenez
Worcester Polytechnic Institute, USA

5:00-5:25 Sea Ice, Climate, and Multiscale Composites
Kenneth M. Golden, University of Utah, USA

5:30-5:55 Identifying the Strongest Composites
Robert P. Lipton, Louisiana State University, USA

6:00-6:25 Optimal Multicomponent Plane Elastic Composites
Andrej V. Cherkaev, University of Utah, USA; Grzegorz Dzierzanowski, Politechnika Warszawska, Poland

6:30-6:55 Fast Algorithms for Mesoscale Evolution of Large Particle Systems
Lyudmyla Barannyk, University of Idaho, USA; Alexander Panchenko, Washington State University, USA

Sunday, June 9

MS21

Vesicles and Inextensible Membranes

5:00 PM-7:00 PM

Room:Aria A - 3rd Floor

Vesicles and inextensible membranes are important components of modern technologies such as directed drug delivery or micro-reactors. Current research in this area includes both analytic and computational approaches to investigate not only the nonlinear dynamics of inextensible membrane systems, but also the dynamics of the membrane composition. This symposium will explore recent numerical tools used to model the dynamics of vesicle flows, the compositional dynamics within lipid bilayer vesicles, and the nonlinear dynamics of inextensible elastic membranes in electric fields. Each of these topics provides insight about these challenging systems.

Organizer: David Salac
University of Buffalo, SUNY, USA

5:00-5:25 Three Dimensional Vesicles in Fluid Flow and Electric Fields: Jump Conditions and a Numerical Method
David Salac, Prerna Gera, and Mohammad Kolahdouz, University of Buffalo, SUNY, USA

5:30-5:55 Compositional Interface Dynamics Within Symmetric and Asymmetric Planar Lipid Bilayer Membranes
Mikko Haataja and Tao Han, Princeton University, USA

6:00-6:25 Nonlinear Dynamics of An Incompressible Elastic Membrane in An Electric Field
Yuan-Nan Young, New Jersey Institute of Technology, USA; Michael Miksis, Northwestern University, USA; Shravan Veerapaneni, University of Michigan, USA; Petia Vlahovska, Brown University, USA

6:30-6:55 Numerical Algorithms for Vesicle Flows
Shravan Veerapaneni, University of Michigan, USA

Sunday, June 9

MS22

Defects and Localized Structures in Thin Elastic Sheets - Part I of II

5:00 PM-7:00 PM

Room:Concerto A - 3rd Floor

For Part 2 see MS40

Thin sheets admit many types of singular, localized structures: Some of which are originated in the microscopic scale of the material, such as creases and crystalline defects; others occur at intermediate scales, such as folds and crumples in confined sheets. The modeling and analysis of those structures, and the possible connections between various localization phenomena is largely virgin territory. This two-part minisymposium highlights some examples, from which a broader understanding is beginning to emerge.

Organizer: Benjamin Davidovitch
University of Massachusetts, Amherst, USA

5:00-5:25 Mechanics of a Folded Elastic Ribbon
Basile Audoly, CNRS and Ecole Polytechnique, France

5:30-5:55 Folding of a Fluid-Supported Sheet
Haim Diamant, Tel Aviv University, Israel

6:00-6:25 First Steps Toward a Multipole Construction of Thin Sheets
Jemal Guven, Universidad Nacional Autónoma de México, Mexico; James A. Hanna, University of Massachusetts, Amherst, USA; Osman Kahraman and *Martin Michael Müller*, Université de Lorraine, Metz, France

6:30-6:55 Wrinkles and Folding on Curved Topographies
Evan Hohlfeld, University of Massachusetts, Amherst, USA

Sunday, June 9

MS23

Analysis and Computations for Non-equilibrium Molecular Systems - Part I of II

5:00 PM-7:00 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS104

The minisymposium will address recent and ongoing developments in analysis and simulation of non-equilibrium molecular systems for materials design. In particular, we will discuss the fidelity and sensitivity of atomistic and coarse-grained stochastic models in transient and stationary regimes. Mathematical topics will include information-theoretic tools, as well as non-equilibrium statistical mechanics techniques and computational methods for analysing driven extended stochastic systems.

Organizer: Markos A. Katsoulakis
University of Massachusetts, Amherst, USA

Organizer: Petr Plechac
University of Delaware, USA

5:00-5:25 Information-theoretic Closures of Moment Hierarchies
Sorin Mitran, University of North Carolina, Chapel Hill, USA

5:30-5:55 Stochastic Methods for Molecular Sampling and Transient Dynamics
Ben Leimkuhler, University of Edinburgh, United Kingdom

6:00-6:25 Information-theoretic Tools for Parametrized Coarse-graining of Non-equlibrium Extended Systems
Petr Plechac, University of Delaware, USA

6:30-6:55 Coarse-Grained Lattice Monte Carlo Simulation of Continuous Systems
Talid Sinno, University of Pennsylvania, USA

Sunday, June 9

MS24

Self-organized Nanostructures in Irradiated Alloys

5:00 PM-7:00 PM

Room:Rhapsody - 4th Floor

In recent years, irradiation by energetic particles has become a promising potential route to self-organized nanofabrication. Significant flexibility in the irradiation environment (ion energy, ion flux, optional material co-deposition, etc..) offers the possibility of tunable synthesis of a variety of nano-scale structural arrays. Although fundamental physical questions remain, recent results indicate that two-component systems offer the most flexibility and promise toward this end. This symposium will highlight current work on ion-irradiated alloys at various scales, combining atomistic simulation, multiscale continuum modeling, and numerical simulation.

Organizer: Scott Norris
Southern Methodist University, USA

5:00-5:25 Self-Assembled Nanoscale Patterns Produced by Ion Bombardment of Two-Component Materials
R. Mark Bradley, Colorado State University, USA

5:30-5:55 Multi-Scale Modeling of Irradiated Alloys: Atomistically-Informed Continuum Models
Scott Norris, Southern Methodist University, USA

6:00-6:25 Spatio-Temporal Self-Organization at the Nanoscale in Alloys Subjected to Sustained Irradiation
Pascal Bellon, Shipeng Shu, Brad Stumphy, and Robert Averback, University of Illinois at Urbana-Champaign, USA

6:30-6:55 Composition Patterning in Irradiation-driven Materials
Anter A. El-Azab, Florida State University, USA; Santosh Dubey, Purdue University, USA

Sunday, June 9

MS25

Modeling and Computations of Liquid Crystal Polymers and Active Nematic Suspensions - Part I of II

5:00 PM-7:00 PM

Room:Minuet - 4th Floor

For Part 2 see MS70

Liquid crystal polymers and active nematic suspensions have attracted much attention in the past because of their wide applications in many environmental and industrial applications. Due to the nonlinear coupling of various complex physical phenomena, their modeling, analysis and numerical simulations are remarkably challenging. The main purpose of this minisymposium is to present some new developments and enhance collaborations in these areas.

Organizer: Ruhai Zhou
Old Dominion University, USA

Organizer: Qi Wang
University of South Carolina, USA

Organizer: Xiaofeng Yang
University of South Carolina, USA

5:00-5:25 Efficient Numerical Schemes for Phase-Field Models of Multiphase Complex Fluids
Jie Shen, Purdue University, USA

5:30-5:55 Mathematical Modeling of Colloids
Maria-Carme Calderer, University of Minnesota, USA

6:00-6:25 Defect Patterns in Liquid Crystal Films
Daniel Phillips, Purdue University, USA

6:30-6:55 Electromagnetic Wave Propagation Through a Liquid Crystal Layer
Hong Zhou, *Eric Choate*, and Michael Winslow, Naval Postgraduate School, USA

Sunday, June 9

MS26

From Microscopic to Continuum: Variational Multiscale Methods: Part I of IV

5:00 PM-7:00 PM

Room:Maestro A - 4th Floor

For Part 2 see MS53

This minisymposium addresses new results in the application of variational multiscale methods to systems related to materials science. Different approaches to coupling of the two extreme scales: the microscopic and the continuum will be at the center of the attention. Other recent advances with mesoscopic and multiscale character, such as: homogenization of composite materials, emergence of wrinkling patterns driven by loading or growth, prediction of dislocations and fracture, dimension reduction, microstructures and thin films of nematic liquid crystal, will be discussed. The objective of this minisymposium is to bring together experts and younger scientists from applied mathematics and mechanics to view advances and challenges from different perspectives.

Organizer: Marta Lewicka
University of Pittsburgh, USA

Organizer: Anja Schloemerkemper
University of Würzburg, Germany

5:00-5:25 About a Γ-Convergence Approach to a Quasicontinuum Method in 1D
Anja Schlömerkemper and Mathias Schäffner, University of Würzburg, Germany

5:30-5:55 Microstructure As a Result of Differential Growth of Thin Films
Peter Bella, Max Planck Institute for Mathematics in the Sciences, Germany; Robert V Kohn, Courant Institute of Mathematical Sciences, New York University, USA

continued on next page

Sunday, June 9

MS26

From Microscopic to Continuum: Variational Multiscale Methods: Part I of IV

continued

6:00-6:25 Continuum Limits of Discrete Dislocation Energies: The Case of the Idealised Pile-up
Lucia Scardia, University of Glasgow, Scotland, UK; Mark Peletier, Ron Peerlings, and Marc Geers, Technische Universiteit Eindhoven, The Netherlands

6:30-6:55 Ambrosio-Tortorelli Approximation for Cavitation
Duvan Henao, UPMC Paris 6, France and Catolica de Chile, Chile; Carlos Mora-Corral, Universidad Autonoma de Madrid, Spain; Xianmin Xu, Chinese Academy of Sciences, China and RWTH Aachen University, Germany

Dinner Break

7:00 PM-8:00 PM

Attendees on their own

Poster Spotlights

8:00 PM-9:00 PM

Room:Symphony - 3rd Floor

Sunday, June 9

PP1

Poster Session

9:00 PM-11:00 PM

Room:Orchestra - 2nd Floor

Algorithm for Linear Programming Involving Interval Constraints
Ibraheem Alolyan, King Saoud University, Saudia Arabia

Constitutive Models for the Macroscopic Response and Microstructure Evolution in Particle-Reinforced Elastomers at Finite Strains
Pedro Ponte Castaneda and *Reza Avazmohammadi*, University of Pennsylvania, USA

Multi Stage Approach to Extract Microstructural Information in X-Ray Microtomography Images: Case Study of Fully Lamellar Titanium Alloy
Laurent Babout, Lukasz Jopek, Michal Postolski, and Marcin Janaszewski, Lodz Technical University, Poland

Quasi-Equilibrium Off-Lattice Kinetic Monte Carlo of Heteroepitaxy
Henry A. Boateng, University of Michigan, USA; Tim Schulze, University of Tennessee, USA; Peter Smereka, University of Michigan, USA

A Second Order Minimality Criterion for Free Discontinuity Problems
Marco Bonacini, SISSA-ISAS International School for Advanced Studies, Italy

A Quantitative Second Order Minimality Criterion for Cavities in Elastic Bodies
Giuseppe Maria Capriani, University of Münster, Germany; Vesa Julin, University of Jyvaskyla, Finland; Giovanni Pisante, Seconda Università degli Studi di Napoli, Italy

Morphological and Mechanical Properties of Entangled Triblock Copolymer Gels
Tanya L. Chantawansri, University of California, Santa Barbara, USA; Timothy Sirk and Yelena Sliozberg, U.S. Army Research Laboratory, USA

continued in next column

Use of Sensitivity Analysis and Error Analysis to Implement Recursively Self-Consistent Programs
Che-Sheng Chung and Sheng-Lyang Jang, National Taiwan University of Science and Technology, Taiwan

A Quasistatic Evolution Model for Perfectly Plastic Plates Derived by Gamma Convergence
Elisa Davoli, Carnegie Mellon University, USA; Maria Giovanna Mora, Università degli Studi di Pavia, Italy

Modeling Collective Chemical Effects in Carbon Nanotube Growth
Brittan A. Farmer, Mostafa Bedewy, and John Hart, University of Michigan, USA

Electro-active Polymer Composites at Finite Deformations: Effective Behavior and Stability Analysis
Morteza Hakimi Siboni and Pedro Ponte Castaneda, University of Pennsylvania, USA

Spectra of Functionalized Operators Arising from Hypersurfaces
Gurgen Hayrapetyan and Keith Promislow, Michigan State University, USA

A Density Result for GSBD and Its Application to the Approximation of Fracture Energies
Flaviana Iurlano, SISSA-ISAS International School for Advanced Studies, Italy

Zero Transmission in Waveguides with Thin Structured Membranes
Jens B. Jorgensen, Courant Institute of Mathematical Sciences, New York University, USA

Tubes of Maximal Probability and Transition Pathway Sampling
Patrick Malsom and Frank Pinski, University of Cincinnati, USA

Mathematical and Computational Methods for the Analysis of Low-Energy Electron Microscopy/ Diffraction of Graphene and Other Semiconductors
John F. Mcclain, University of New Hampshire, USA; Jiebing Sun, Michigan State University, USA; James Hannon, IBM T.J. Watson Research Center, USA; Karsten Pohl and Jian-Ming Tang, University of New Hampshire, USA

continued on next page

Mystic and Uncertainty Quantification in Materials Design, Analysis, and Failure
Michael McKerns, and Houman Owhadi, California Institute of Technology, USA; Tim Sullivan, University of Warwick, United Kingdom; Alta Fang, Princeton University, USA; Michael Aivazis, California State University, USA

Renormalized Energy and Dynamics of Screw Dislocations with Antiplane Shear
Marco Morandotti, Timothy Blass, Irene Fonseca, and Giovanni Leoni, Carnegie Mellon University, USA

On Modeling Plane-Strain Fracture Using Strain-Limiting Theory of Elasticity
Mallikarjunaiah S. Muddamallappa, Texas A&M University, USA

Connection of Kinetic Monte Carlo Method for Surfaces to the Burton-Cabrera-Frank Model
Paul Patrone, University of Maryland, College Park and National Institute of Standards and Technology (NIST), USA; Dionisios Margetis, University of Maryland, College Park, USA

Evolution Results for Epitaxially Strained Thin Films
Paolo Piovano, CNR-IMATI, Pavia, Italy

A Model for Crack Growth with Branching and Kinking
Simone Racca, SISSA-ISAS International School for Advanced Studies, Italy

Behavioral Modeling of Corundum under the Effect of Porosity Rate
Bendaoudi Seifeddine, Bounazef Mokhtar, and Adda Bedia El-Abbes, Djillali Liabes University of Sidi Bel Abbes, Algeria

continued in next column

Practical Modelling of Statistical Nanocomposite Optical Coating Materials for Filter and Absorber Specifications: Oscillator Model, Mixing Model and Spectral Moments Approaches
Olaf Stenzel and Steffen Wilbrandt, Fraunhofer Institute Jena, Germany; Karen Köhler, Bonn University, Germany; Norbert Kaiser, Fraunhofer Institute Jena, Germany

Nonlinear Solvers for Dislocation Dynamics
Carol S. Woodward, Athanasio Arsenlis, Sylvie Aubry, Gregg Hommes, and Moono Rhee, Lawrence Livermore National Laboratory, USA

Domain Wall Motion in Magnetic Nanowires: An Asymptotic Approach
Ross Lund, University of Bristol, United Kingdom; Arseni Goussev, Northumbria University, United Kingdom; Jonathan Robbins, Valeriy Slastikov, and Charles Sonnenberg, University of Bristol, United Kingdom

Collective Behavior of Walls of Dislocations
Patrick van Meurs, Eindhoven University of Technology, Netherlands

Electron Transport in Thin Semiconductor Gas Sensors
Hechmi Hattab, ENIT-LAMSIN, Tunisia

Monday, June 10

Registration
7:30 AM-5:30 PM
Room:Overture - 3rd Floor

Remarks
8:00 AM-8:15 AM
Room:Symphony - 3rd Floor

IP4

Scaling in Kinetic Mean-field Models for Coarsening Phenomena
8:15 AM-9:00 AM
Room:Symphony - 3rd Floor
Chair: Peter Voorhees, Northwestern University, USA

Coarsening, that is the increase of typical length scales in a microstructure, plays a crucial role in the large-time behavior of numerous processes in physics and materials science. An important aspect is the dynamical scaling hypothesis suggesting that after some transient regime the system evolves in a universal statistically self-similar fashion. Kinetic mean-field models are often used to try to capture this self-similar behavior. However, despite typically simple looking, their analysis turns out to be a challenge. In this talk I will review the progress of recent years in the analysis of such equations and will also discuss major open problems.

Barbara Niethammer
University of Bonn, Germany

Monday, June 10

IP5

Numerical Methods in Molecular Dynamics

9:00 AM-9:45 AM

Room:Symphony - 3rd Floor

Chair: Mitchell Luskin, University of Minnesota, USA

Molecular dynamics is now a very widely used tool to study the matter at the molecular level. It is used in various fields, such as biology, chemistry or materials science. The aim is in particular to understand the relationships between the macroscopic properties of a molecular system and its atomistic features. For example, one would like to compute the constitutive relations for materials from molecular models, or predict the most likely conformations of a protein in a solvent from its amino acid sequence. One of the difficulty to reach this aim is related to timescales: the typical timescale of a molecular dynamics simulation is much smaller than the typical timescale at which the crucial events, from a macroscopic viewpoint, occur. This is related to the metastability of a molecular dynamics trajectory: the system stays for a very long time in some regions of the configuration space (called metastable state), before hopping to another one, and it is difficult to observe and simulate such rare events. An associated feature is the multimodality of the statistical ensemble (a probability measure) sampled by the molecular dynamics trajectories. Many methods have been proposed in the molecular dynamics community to deal with these difficulties, and we will focus on two prototypical ones for which a mathematical analysis gives useful insights. We will first present adaptive importance sampling techniques, which have been proposed to sample efficiently statistical ensembles. Then, we will propose a mathematical analysis of the parallel replica algorithm which has been introduced by A.F. Voter to generate efficiently metastable dynamics.

Tony Lelievre
CERMICS ENPC, France

Monday, June 10

Coffee Break

9:45 AM-10:15 AM

Room:Assembly - 3rd Floor

Monday, June 10

MS28

Aspects of Homogenization: Analysis and Applications - Part II of II

10:15 AM-12:15 PM

Room:Symphony - 3rd Floor

For Part 1 see MS19

In the last few decades, numerous studies have focused on the relationship between microscopic descriptions of large systems and the overall effective (e.g., elastic, thermal, electrical) parameters that govern the system macroscopic behavior. Applications range from models of dislocation dynamics in solids to the design of optimal high-performance composites and metamaterials to the characterization of effective properties of biological and biophysical systems. With this minisymposium, we aim to bring together experts in homogenization who work on diverse problems related to Materials Science and Biophysics. A goal is to identify emergent approaches and discuss results that shed light on properties of complex systems.

Organizer: Dionisios Margetis
University of Maryland, College Park, USA

Organizer: Antoine Mellet
University of Maryland, USA

10:15-10:40 Spectral Representation and Evolution of Microstructure
Elena Cherkaev, University of Utah, USA

10:45-11:10 Double Negative Behavior in Metamaterials and Multi-Scale Analysis
Robert P. Lipton, Louisiana State University, USA

11:15-11:40 Models and Analysis for Cohesive Dynamic Fracture
Christopher Larsen, Worcester Polytechnic Institute, USA

11:45-12:10 Large Deviations, Metastability and Monte Carlo Methods for Multiscale Problems
Konstantinos Spiliopoulos, Boston University, USA; Paul Dupuis and Hui Wang, Brown University, USA

Monday, June 10

MS29

Theoretical Modeling and Applications of Metamaterials - Part I of IV

10:15 AM-12:15 PM

Room:Aria B - 3rd Floor

For Part 2 see MS38

Dense arrays of resonant inclusions, or other substructures formed from high contrast constituents, can provide exciting bulk electromagnetic, elastodynamic, and acoustic properties that are not available in any of their constituent elements. Modeling these 'meta-' effects can become particularly challenging, especially in frequency regions in which the most interesting phenomena arise. Consequently, conventional established tools from material science need to be properly corrected and improved to rigorously capture the physics and phenomena underlying these effects. This minisymposium highlights the most recent advances in mathematical modeling, physical understanding and applications of metamaterials and their impact on the theory and applications of material science and engineering.

Organizer: Andrea Alu
University of Texas at Austin, USA

Organizer: Graeme W. Milton
University of Utah, USA

10:15-10:40 Physical Bounds, Potentials and Fundamental Limitations of Metamaterial Cloaks
Andrea Alu and Francesco Monticone, University of Texas at Austin, USA

10:45-11:10 Radiationless Electromagnetic Modes in Open Plasmonic Nanostructures
Mario Silveirinha, University of Coimbra, Portugal

11:15-11:40 Branch-cuts and Sharp Corners in Composite Inclusions
Ross McPhedran, University of Sydney, Australia

11:45-12:10 Towards Digital Metamaterials
Cristian Della Giovampaola and *Nader Engheta*, University of Pennsylvania, USA

Monday, June 10

MS30

Multiscale Computation of Fluctuating Hydrodynamics and Microscale Mechanics - Part II of III

10:15 AM-12:15 PM

Room:Aria A - 3rd Floor

For Part 1 see MS3
For Part 3 see MS57

The hydrodynamics of complex fluids, such as polymer solutions, colloidal suspensions and reactive fluid mixtures, has recently attracted great interest. Coarse-grained models cover a broad range of time and length scales by incrementally sacrificing physical fidelity for computational efficiency. This minisymposium will focus on advances in multiscale numerical methods for simulating flows and biomechanical structures at mesoscopic scales. Issues to be discussed will cover the inclusion of thermal fluctuations in analytical and computational models, coupling of continuum fluids to immersed structures and calibration of effective parameters.

Organizer: Christel Hohenegger
University of Utah, USA

Organizer: Scott McKinley
University of Florida, USA

Organizer: Aleksandar Donev
Courant Institute of Mathematical Sciences, New York University, USA

10:15-10:40 The Micromechanics of Colloidal Dispersions
John F. Brady, California Institute of Technology, USA

10:45-11:10 Biofilm Streamers in Porous Environments
Howard A. Stone, Princeton University, USA

11:15-11:40 Statistical Analysis of Passive Particle Tracking in Microrheology
Natesh Pillai, Harvard University, USA

11:45-12:10 Collective Dynamics in Suspensions of Motile Micro-particles
Enkeleida Lushi, Imperial College London, United Kingdom and Courant Institute of Mathematical Sciences, New York University, USA

Monday, June 10

MS31

Metric-driven Deformation of Thin Elastic Sheets - Part II of III

10:15 AM-12:15 PM

Room:Concerto A - 3rd Floor

For Part 1 see MS4
For Part 3 see MS58

The shape of a thin sheet in R^3 reflects its preference for isometric embedding, and its resistance to bending. When the sheet is Euclidean, isometric embeddings are developable surfaces. But non-Euclidean sheets occur in nature (due to differential growth) and can also be created in the laboratory. We are just beginning to understand how the sheet's metric and its mechanical properties conspire to determine the shape it assumes in space. This 3-part minisymposium highlights the area's interdisciplinary character, combining geometry with analysis, physics with mathematics, and experiment with theory.

Organizer: Robert V. Kohn
Courant Institute of Mathematical Sciences, New York University, USA

10:15-10:40 Nonlinear Structure and Mechanics of Filament Bundles: Intrinsic Geometry of Twist and Defect-Riddled Ground States
Gregory M. Grason, University of Massachusetts, Amherst, USA

10:45-11:10 A Riemannian Approach to Dimension Reduction in Non-Euclidean Elasticity
Cy Maor, Raz Kupferman, and Jake Solomon, Hebrew University, Israel

11:15-11:40 How to Derive Equilibrium Equations for Fully Nonlinear Bending Theories in Euclidean and Non-Euclidean Elasticity
Peter Hornung, Max Planck Institute for Mathematics in the Sciences, Germany

11:45-12:10 Riemannian Analysis of Pre-stressed Elastic Materials
Raz Kupferman, Hebrew University, Israel

Monday, June 10

MS32

Micro-to-Macro Coarse-Graining and Effective Dynamics in Nonequilibrium Systems - Part II of III

10:15 AM-12:15 PM

Room:Concerto B - 3rd Floor

For Part 1 see MS5
For Part 3 see MS59

This symposium will bring together speakers who work on Nonequilibrium problems related to materials at various lengthscales ranging from atomic to polycrystalline.

Organizer: Kaushik Dayal
Carnegie Mellon University, USA

10:15-10:40 A Theory and Challenges for Coarsening in Microstructure
David Kinderlehrer, Carnegie Mellon University, USA; Katayun Barmak, Columbia University, USA; Eva Eggeling, Fraunhofer Institute for Computer Graphics, Germany; Maria Emelianenko, George Mason University, USA; Yekaterina Epshteyn, University of Utah, USA; Richard Sharp, Microsoft Corporation, USA; Shlomo Ta'asan, Carnegie Mellon University, USA

10:45-11:10 Mathematical Challenges in Interpretation of Hedm Data
Shlomo Ta'asan, Carnegie Mellon University, USA

11:15-11:40 Multiscale Modeling of Ge Nano-Crystallization from Amorphous Phase
Celia Reina, University of Pennsylvania, USA; Luis Sandoval and Jaime Marian, Lawrence Livermore National Laboratory, USA

11:45-12:10 Critical Aspect Ratio in a Single Crystal Shear Experiment
Patrick Dondl, Durham University, United Kingdom

Monday, June 10

MS33

Recent Developments in Modeling Crystallization and Material Properties with Periodic Fields - Part II of III

10:15 AM-12:15 PM

Room:Rhapsody - 4th Floor

For Part 1 see MS6
For Part 3 see MS69

Employing free energy functionals that are minimized by periodic fields allows one to study a variety of phenomena including nucleation and growth, epitaxial growth, yield strength of polycrystals, grain boundary melting and glass formation. This approach is the basis of dynamical classical density functional theory and phase field crystal models. There has been tremendous activity in this field including applications in liquid crystals, ordering on curved surfaces and hydrodynamic/crystal interaction. This minisymposium will explore recent advances in three major avenues namely specific applications in material science, extensions to more complex systems and the connection between various approaches and traditional methods.

Organizer: Arvind Baskaran
University of California, Irvine, USA

Organizer: Ken Elder
Oakland University, USA

Organizer: John Lowengrub
University of California, Irvine, USA

10:15-10:40 Particles at Fluid-fluid Interfaces: A New Navier-Stokes-Cahn-Hilliard Surface Phase-Field Crystal Model
John Lowengrub, University of California, Irvine, USA

10:45-11:10 Phase Field Crystal Models of Grain Growth
Peter Voorhees and Kuo-An Wu, Northwestern University, USA; Edwin Schwalbach and James Warren, National Institute of Standards and Technology, USA

continued in next column

11:15-11:40 Phase Field Crystal Modeling of Microstructure in Multi-Component Alloys
Nikolas Provatas, McGill University, Canada

11:45-12:10 Modeling Defect Structures and Associated Slow Processes in 3D Materials with Phase Field Crystal Methods
Joel Berry, McMaster University, Canada; Nikolas Provatas, McGill University, Canada; Joerg Rottler, University of British Columbia, Canada; Chad W. Sinclair, University of British Columbia, Canada

Monday, June 10

MS34

The Ginzburg-Landau Model and Related Topics - Part II of V

10:15 AM-12:15 PM

Room:Minuet - 4th Floor

For Part 1 see MS7
For Part 3 see MS61

The focus of the minisymposium is on mathematical problems related to Ginzburg-Landau model with application in physics and materials science including but not limited to: superconductivity, superfluidity, liquid crystals, and polymers. The speakers in this minisymposium will describe their recent research including the development and structure of singular solutions of the Ginzburg-Landau-type problems and the dynamics of vortex motion.

Organizer: Yaniv Almog
Louisiana State University, USA

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Leonid Berlyand
Pennsylvania State University, USA

10:15-10:40 Vortex Dynamics with Pinning and Strong Fields
Ian Tice, Brown University, USA; Sylvia Serfaty, Universite Pierre et Marie Curie (Paris 6), France

10:45-11:10 Equidistribution Results for the Renormalized Energy and 2D Coulomb Gases
Sylvia Serfaty, Universite Pierre et Marie Curie (Paris 6), France; Simona Rota Nodari, Universite de Cergy-Pontoise, France

11:15-11:40 Analysis of Two-Dimensional Phases in Bent-Core Liquid Crystals
Tiziana Giorgi, New Mexico State University, USA

11:45-12:10 On the Nature of Defects in the Q-Tensor Theory of Nematic Liquid Crystals
Arghir Zarnescu, University of Sussex, United Kingdom

Monday, June 10

MS35

Electronic Structure - Part II of IV

10:15 AM-12:15 PM

Room:Maestro A - 4th Floor

For Part 1 see MS8
For Part 3 see MS62

Predicting the elctronic structure of complex molecular and condensed-matter systems has been a focus of attention in chemistry and physics for decades. More recently, espceically since the advent of density functional theory (DFT), it has also become an important ingredient in materials science. Electronic structure models allows the on-the-fly computation of non-empirical and chemically specific interatomic interactions within larger-scale simulations.

Organizer: Gero Friesecke
Technische Universität München, Germany

Organizer: Eric Cances
Ecole des Ponts and INRIA, France

Organizer: Lin Lin
Lawrence Berkeley National Laboratory, USA

Organizer: Chao Yang
Lawrence Berkeley National Laboratory, USA

10:15-10:40 Fast Numerical Methods for Electronic Structure Calculations
Lin Lin, Lawrence Berkeley National Laboratory, USA

10:45-11:10 Many-Body Propagators and the GW Approximation of the Self-Energy Operator
Fang Liu, Lawrence Livermore National Laboratory, USA; Lin Lin and Chao Yang, Lawrence Berkeley National Laboratory, USA

11:15-11:40 Exciton Diffusion in Organic Solar Cells: First--Principles Investigations
Gang Lu, Xu Zhang, and Zi Li, California State University, Northridge, USA

11:45-12:10 Fixed-Point Optimization of Atoms and Density in Dft
Laurence Marks, Northwestern University, USA

Monday, June 10

MS36

Mathematical Crystallography: Beyond Classical Crystal Symmetry - Part II of III

10:15 AM-12:15 PM

Room:Maestro B - 4th Floor

For Part 1 see MS9
For Part 3 see MS90

Generalizating the classical crystalline symmetries is a key path for understanding complex structural relations as well as designing new materials in crystal engineering. This path includes searching for common principles linking apparently unrelated structures and governing the mechanisms of phase transitions and the analysis of aperiodic, quasi-periodic, para-crystalline, and other not-quite-crystals. These have inspired variants and generalizations of the periodic arrays of traditional crystals. This is part exploration: what novel kinds of objects can be discovered, synthesized, or represented? This is part analysis: what are these objects, how good are our representations, and how do we make sense of them?

Organizer: Gregory McColm
University of South Florida, USA

Organizer: Massimo Nespolo
Université de Lorraine, France

10:15-10:40 A Stroll Along Structural Paths: Symmetry, Pseudo-Symmetry and Their Exploitation to Understand and Design Structures
Massimo Nespolo, Université de Lorraine, France

10:45-11:10 Recent Advances in Mathematical Diffraction Theory
Uwe Grimm, The Open University, United Kingdom

11:15-11:40 Periodicity, Aperiodicity and Prehistory
Marjorie Senechal, Smith College, USA

11:45-12:10 Coincidence Site Lattices and Well-rounded Sublattices in the Plane
Peter Zeiner, University of Bielefeld, Germany

Lunch Break

12:15 PM-1:30 PM

Attendees on their own

Monday, June 10

IP6

Tracking Multiphase Physics: Geometry, Foams, and Thin Films

1:30 PM-2:15 PM

Room:Symphony - 3rd Floor

Chair: Greg Forest, University of North Carolina at Chapel Hill, USA

Many scientific and engineering problems involve interconnected moving interfaces separating different regions, including dry foams, crystal grain growth and multi-cellular structures in man-made and biological materials. Producing consistent and well-posed mathematical models that capture the motion of these interfaces, especially at degeneracies, such as triple points and triple lines where multiple interfaces meet, is challenging. Joint with Robert Saye of UC Berkeley, we introduce an efficient and robust mathematical approach to computing the solution to two and three-dimensional multi-interface problems involving complex junctions and topological changes in an evolving general multiphase system. We demonstrate the method on a collection of problems, including geometric coarsening flows under curvature, incompressible flow coupled to multi-fluid interface problems, and (joint with C. Rycroft), the interaction of growing biological clusters with elastic basement membranes. Finally, we compute the dynamics of unstable foams, such as soap bubbles, evolving under the combined effects of gas-fluid interactions, thin-film lamella drainage, and topological bursting.

James Sethian
University of California, Berkeley, USA

Intermission

2:15 PM-2:30 PM

Monday, June 10

MS37

Homogenization and Applications - Part II of III

2:30 PM-4:30 PM

Room:Symphony - 3rd Floor

For Part 1 see MS10
For Part 3 see MS55

This minisymposium proposal is concerned with recent developments in homogenization and its applications for modeling and understanding the overall response of various types of heterogeneous material systems. The specific topics include nonlinear constitutive behaviors, including finite elasticity and plasticity, as well as coupled properties, including applications to elasto-plastic behavior, ferroelectric and thermoelectric composites, and shape memory polycrystals. In addition, the MS includes presentations dealing with recent advances on universal bounds, instabilities for nematic liquid crystal elastomers, atomistic-to-continuum multi-scale modeling and phononic transport. The 12 presentations are organized in 3 sessions as follows (presenters are shown in boldface).

Organizer: Pedro Ponte Castaneda
University of Pennsylvania, USA

Organizer: Pierre M. Suquet
CNRS, France

2:30-2:55 On the Coupling Between Transformation and Plasticity in Polycrystals

Kaushik Bhattacharya, California Institute of Technology, USA

3:00-3:25 Nonlinear Asymptotic Homogenization of Thermoelectric Composites

Yang Yang and *Jiangyu Li*, University of Washington, USA

continued in next column

3:30-3:55 Continuum Electromechanical Theory for Nematic Continua with Applications to Freedericksz Instability

Nicolas Triantafyllidis, Ecole Polytechnique, Palaiseau, France; Gianpiero Pampolini, École Polytechnique, France

4:00-4:25 Constitutive Models for Magneto-Active Elastomers at Finite Strains

Pedro Ponte Castañeda, University of Pennsylvania, USA

Monday, June 10

MS38

Theoretical Modeling and Applications of Metamaterials - Part II of IV

2:30 PM-4:30 PM

Room:Aria B - 3rd Floor

For Part 1 see MS29
For Part 3 see MS83

Dense arrays of resonant inclusions, or other substructures formed from high contrast constituents, can provide exciting bulk electromagnetic, elastodynamic, and acoustic properties that are not available in any of their constituent elements. Modeling these 'meta-' effects can become particularly challenging, especially in frequency regions in which the most interesting phenomena arise. Consequently, conventional established tools from material science need to be properly corrected and improved to rigorously capture the physics and phenomena underlying these effects. This minisymposium highlights the most recent advances in mathematical modeling, physical understanding and applications of metamaterials and their impact on the theory and applications of material science and engineering.

Organizer: Andrea Alu
University of Texas at Austin, USA

Organizer: Graeme W. Milton
University of Utah, USA

2:30-2:55 Causality of the Inverse of Causal Constitutive Parameters for Natural Materials and Metamaterials
Arthur D. Yaghjian, Electromagnetics Research Consultant, USA

3:00-3:25 Lagrangian Treatment of Systems Composed of High-Loss and Lossless Components
Alexander Figotin, University of California, Irvine, USA; Aaron Welters, Massachusetts Institute of Technology, USA

continued in next column

3:30-3:55 On the Sensitivity of the Annomallous Localized Ressonance Phenomenon to Small Variations in the Loss Level
Daniel Onofrei, University of Houston, USA

4:00-4:25 Optical Topological Insulators and Spin-cloaking Based on bi-anisotropic Metamaterials
Gennady Shvets, University of Texas at Austin, USA

Monday, June 10

MS39

Motility and Mechanics of Biomolecular Complexes - Part I of III

2:30 PM-4:30 PM

Room:Aria A - 3rd Floor

For Part 2 see MS66

This symposium will focus on problems which draw on ideas from solid, fluid and statistical mechanics. Problems in soft materials, elastomers and biophysics are already of this nature. But, we anticipate that areas such as, complex fluids, mechanics of self-propulsion, etc., where there is significant overlap with chemistry can also benefit from mathematical approaches where Brownian motion is accounted for. Some representative topics in this symposium include: (a) Fluctuating rod models for biopolymers, (b) Mechanics of force generation in cells, (c) Swimming and self-propulsion in complex fluids, (d) Coarse-grained simulations of cellular organelles, (e) Phase transitions in macromolecular complexes.

Organizer: Prashant K. Purohit
University of Pennsylvania, USA

Organizer: Antonio De Simone
SISSA, Italy

2:30-2:55 Torsion of Fluctuating DNA
Prashant K. Purohit, University of Pennsylvania, USA

3:00-3:25 A Sequence-dependent Rigid Base Model of DNA, and its Continuum Birod Limit
John H. Maddocks, École Polytechnique Fédérale de Lausanne, Switzerland

3:30-3:55 The Chemo-mechanics of Cytoskeletal Force Generation
Krishna Garikipati, University of Michigan, Ann Arbor, USA

4:00-4:25 Coarse-grained Molecular Dynamics Modeling of the Disordered Domain of Nuclear Pores
Ali Ghavami and Erik van der Giessen, University of Groningen, Netherlands; Patrick Onck, University of Groningen, The Netherlands

Monday, June 10

MS40

Defects and Localized Structures in Thin Elastic Sheets - Part II of II

2:30 PM-4:30 PM

Room:Concerto A - 3rd Floor

For Part 1 see MS22

Thin sheets admit many types of singular, localized structures: Some of which are originated in the microscopic scale of the material, such as creases and crystalline defects; others occur at intermediate scales, such as folds and crumples in confined sheets. The modeling and analysis of those structures, and the possible connections between various localization phenomena is largely virgin territory. This two-part minisymposium highlights some examples, from which a broader understanding is beginning to emerge.

Organizer: Benjamin Davidovitch
University of Massachusetts, Amherst, USA

2:30-2:55 Disclination Induced Wrinkles in Free Standing Smectic Membranes
Elisabetta Matsumoto, Princeton University, USA; Nicolás García and Daniel A. Vega, Universidad Nacional del Sur, Argentina

3:00-3:25 Computational Crumpling via Discrete Developable Surfaces
Etienne Vouga, Columbia University, USA; Max Wardetzky, University of Goettingen, Germany; Eitan Grinspun, Columbia University, USA

3:30-3:55 Elastic Concertina and Tearing of Sheets
Eugenio Hamm, Universidad de Santiago de Chile, Chile

4:00-4:25 Geometry of a Crumpled Sheet
Narayanan Menon, University of Massachusetts, Amherst, USA

Monday, June 10

MS41

Computational Tools for Metastable Systems - Part II of III

2:30 PM-4:30 PM

Room:Concerto B - 3rd Floor

For Part 1 see MS14
For Part 3 see MS77

Many materials, including crystals, metals and biological media, possess metastable states that introduce a severe time scale separation. Consequently, direct numerical simulations may be unable to observe important transitions, such as the migration of a defect through a crystal or the folding of a protein. A variety of techniques have been proposed to accelerate these computations, including accelerated dynamics and kinetic Monte Carlo. In this minisymposium, we present recent advances and analysis of such techniques.

Organizer: Gideon Simpson
University of Minnesota, USA

Organizer: Jonathan Weare
University of Chicago, USA

Organizer: Arthur F. Voter
Los Alamos National Laboratory, USA

Organizer: Mitchell Luskin
University of Minnesota, USA

2:30-2:55 Transition Path Sampling
Frank Pinski, University of Cincinnati, USA

3:00-3:25 A Micro / Macro Parareal Algorithm for a Class of Multiscale-in-time Systems
Frederic Legoll, Ecole Nationale des Ponts et Chaussées, France

3:30-3:55 Reaction Pathways of Metastable Markov Chains with Application to Lennard-Jones Clusters Reorganization
Eric Vanden Eijnden, Courant Institute of Mathematical Sciences, New York University, USA

4:00-4:25 Rare Event Simulations for Systems Far from Equilibrium
Aaron Dinner, University of Chicago, USA

Monday, June 10

MS42

Parsing Experimental and Simulation Data: Pattern Extraction, Analysis, and Reproduction - Part II of II

2:30 PM-4:30 PM

Room:Rhapsody - 4th Floor

For Part 1 see MS15

New simulation and data acquisition techniques in materials science provide us with large amounts of raw data that represent materials on scales ranging from the mesoscopic to the atomistic. Consequently, the issues of how to: (1) extract and represent the mesoscopic material structure, (2) understand and represent this structure in terms of appropriate statistical descriptors, and (3) generate new raw data which is faithful to such statistical descriptors in order to perform further numerical studies must be addressed in order to allow for model validation or the analysis of material behavior. The minisymposium discusses mathematical methods related to these issues.

Organizer: Benedikt K. Wirth
Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Matt Elsey
Courant Institute of Mathematical Sciences, New York University, USA

2:30-2:55 Modeling Heterogeneous Materials via Lower-order Spatial Correlation Functions Extracted from Limited Experimental Data
Yang Jiao, Princeton University, USA

3:00-3:25 Finding Order in Disorder: Shape Matching and Other Tricks
Sharon C. Glotzer, University of Michigan, USA

3:30-3:55 Analyzing Upper Tails of Grain Size Distributions Using Extreme Value Theory
Sean Donegan and Anthony Rollett, Carnegie Mellon University, USA

4:00-4:25 Fast Automated Detection of Crystal Distortion and Crystal Defects in Polycrystal Images
Matt Elsey and *Benedikt K. Wirth*, Courant Institute of Mathematical Sciences, New York University, USA

Monday, June 10

MS43

Mathematical Advances in Liquid Crystals - Part II of II

2:30 PM-4:30 PM

Room:Minuet - 4th Floor

For Part 1 see MS16

Liquid crystals are a state of matter intermediate between an isotropic liquid and a crystalline solid in that they are uniquely characterized by orientational order and possibly some positional order. They are widely used in the display industry and are good candidates for other applications such as optical metamaterials, actuators and sensors. The aim of this minisymposium is to gather scientists from around the world to discuss modeling, analysis, and simulations of liquid crystalline materials as well as related experimental results. Among other issues, the speakers will describe their recent work in liquid crystal suspensions, hydrodynamics, materials forming quasicrystals, etc.

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Xiaoyu Zheng
Kent State University, USA

2:30-2:55 Efficient Energy Stable Numerical Schemes and Simulations of Two Phase Complex Fluids on Phase Field Method
Xiaofeng Yang, University of South Carolina, USA

3:00-3:25 Liquid Crystals: Revisiting Kinetic Equations and Picking the Best Order Parameters
Ibrahim Fatkullin, University of Arizona, USA

3:30-3:55 Chevron-Like Defects in Smectic Liquid Crystals
Daniel Phillips, Purdue University, USA; Lei Cheng, Indiana University Kokomo, USA

4:00-4:25 Analysis of Liquid Crystal Phase Transitions in Biological Networks
Maria-Carme Calderer, University of Minnesota, USA

Monday, June 10

MS44

Mathematical Aspects of Singularity Formation in Thin Liquid Flows - Part II of II

2:30 PM-4:30 PM

Room:Maestro A - 4th Floor

For Part 1 see MS17

Liquid films of micro- or nanoscale thickness occur widely in nature and industrial processes such as e.g. printing, spraying and electrowetting. Their qualitative behavior differs substantially from the behavior on larger scales since the interplay between surface tension and other intermolecular interactions becomes important. Rupture or coalescence of thin films as well as motion of contact lines typically lead to the formation of singularities in the pressure or liquid profile. The minisymposium provides a platform to investigate these singularities from an analytical, numerical and modeling perspective.

Organizer: Hans Knuepfer

University of Bonn, Germany

Organizer: Georgy Kitavtsev
Max Planck Institute for Mathematics in the Sciences, Germany

2:30-2:55 Boundary Conditions for the Moving Contact Line Problem and the Spreading of Thin Films
Weiqing Ren, National University of Singapore and IHPC, Singapore

3:00-3:25 Electrostatically Induced Singular Dynamics in Long-Wave Annular Film Flows
Alexander Wray, Imperial College of London, United Kingdom

3:30-3:55 Thin Film Models of Liquid Displacement on Chemically Patterned Surfaces for Lithographic Printing Processes
Satish Kumar, University of Minnesota, USA

4:00-4:25 Capillary Fracture of Soft Gels
Joshua Bostwick, Mark Shillaci, and Karen Daniels, North Carolina State University, USA

Monday, June 10

MS45

Nonlinear Lattice Dynamics - Part II of III

2:30 PM-4:00 PM

Room:Maestro B - 4th Floor

For Part 1 see MS18
For Part 3 see MS63

Many problems in materials science concern phenomena where an interplay between discreteness and dynamics plays a fundamental role. Examples include propagation of defects, pattern formation and emergence of complexity and the application range from metamaterials to granular media. The main mathematical issues concern interaction between nonlinearity and dispersion, extremely ragged energy landscapes, trapping, depinning and radiative damping. This minisymposium features talks by leading experts in nonlinear lattice dynamics and aims at facilitating the exchange of ideas and at highlighting the most important unsolved problems in this field.

Organizer: Anna Vainchtein
University of Pittsburgh, USA

Organizer: Lev Truskinovsky
Ecole Polytechnique, France

2:30-2:55 The p-Schrödinger Equation and Granular Crystals
Brigitte Bidégaray-Fesquet, Eric Dumas, and *Guillaume James*, Université de Grenoble and CNRS, France

3:00-3:25 On the Nonlinear Dynamics of Granular Lattices
Fernando Fraternali, University of Salerno, Italy

3:30-3:55 Inertia-Induced Criticality in Martensites
Lev Truskinovsky, Ecole Polytechnique, France

Coffee Break

4:30 PM-5:00 PM

Room:Assembly - 3rd Floor

Monday, June 10

MS46

Stochastic Homogenization: Quantitative Theory and Application to Materials Science - Part II of II

5:00 PM-7:00 PM

Room:Symphony - 3rd Floor

For Part 1 see MS1

Homogenization theory for PDEs with random coefficients can been used to characterize the bulk properties of a material having random microstructural properties. These two sessions explore recent theoretical and computational advances in homogenization theory for stochastic equations. In particular, they focus on a quantitative version of the theory (including fluctuation and error estimation), on efficient numerical computation tools, and on novel applications to materials.

Organizer: Antoine Gloria
Université Libre de Bruxelles, Belgium

Organizer: James Nolen
Duke University, USA

5:00-5:25 From Polymer Physics to Rubber Elasticity: a Stochastic Homogenization Approach
Antoine Gloria, Université Libre de Bruxelles, Belgium

5:30-5:55 Effective Behavior of Interfaces in a Random Elastic Medium
Patrick Dondl, Durham University, United Kingdom

6:00-6:25 Macro and Micro-Based Solutions for Random Heterogeneous Microstructures
Mircea Grigoriu, Cornell University, USA

6:30-6:55 On a Class of "weakly" Stochastic Problems Amenable to Rapid Computational Approaches in Stochastic Homogenization
Claude Le Bris, Ecole Nationale des Ponts et Chaussées, France

Monday, June 10

MS47

Multiscale Modeling, Microstructure, and Local Field Properties of Heterogeneous Media - Part III of III

5:00 PM-7:00 PM

Room:Aria B - 3rd Floor

For Part 2 see MS20

The special session is aimed at presenting recent developments concerning the "micro-macro" interconnection in heterogeneous materials. The session will bring together experts that will focus on the recent developments and current challenges in the homogenization of partial differential equations with oscillatory coefficients, fine-scale stress concentration modeling, nonlocal continuum modeling, peridynamics, complexity reduction and multiscale computational modeling with applications to composites, suspensions, and biomaterials.

Organizer: Lyudmyla Barannyk
University of Idaho, USA

Organizer: Yuliya Gorb
University of Houston, USA

Organizer: Silvia Jimenez
Worcester Polytechnic Institute, USA

5:00-5:25 Model Reduction and Recovery of Structural Information in Heterogeneous Materials
Elena Cherkaev, University of Utah, USA

5:30-5:55 The Underlying Analytical Links Between Various Effective Coefficients of a Poroelastic Medium: a Dehomogenization Approach
Miao-Jung Yvonn Ou, University of Delaware, USA

6:00-6:25 Scattering and Resonances of Electromagnetic Waves by Thin High Contrast Dielectric Structures
Shari Moskow and David Ambrose, Drexel University, USA

6:30-6:55 Approximation of DtN Map in a High Contrast Conductivity Problem
Yuliya Gorb, University of Houston, USA; Liliana Borcea and Yingpei Wang, Rice University, USA

Monday, June 10

MS48

Complex Fluids: Modeling and Simulation - Part II of II

5:00 PM-6:30 PM

Room:Aria A - 3rd Floor

For Part 1 see MS12

Complex fluids are materials with a complicated microstructure, materials that can exhibit both viscous and elastic behavior, for example polymer and colloidal solutions. Properties of these fluids can be exploited to produce materials useful in industrial (soaps and gels) and biological (blood flow and drug delivery) applications. The physics and dynamics of complex fluids are nontrivial, requiring detailed modeling combined with intricate analytic and simulation methods. The goal of this symposium is to bring together mathematicians and practitioners in the area to advance the subject through discussion and collaboration.

Organizer: Michael Cromer
University of Delaware, USA

Organizer: Lin Zhou
New York City College of Technology, USA

5:00-5:25 A General Constitutive Framework for Modeling Elasto-Visco-Plastic Behavior, Yielding and Thixotropy in Waxy Crude-Oils, Microgels and Other Soft Solid Materials
Gareth H. McKinley, Massachusetts Institute of Technology, USA

5:30-5:55 Modeling and Simulation of Complex Biological Fluids Biofilms
Qi Wang and Jia Zhao, University of South Carolina, USA

6:00-6:25 Mathematical Modeling of the Mucus Barrier in Human Lungs
Paula A. Vasquez, Greg Forest, David Hill, and Yuan Jin, University of North Carolina at Chapel Hill, USA

Monday, June 10

MS49

Stress-induced Wrinkling of Thin Elastic Sheets - Part II of II

5:00 PM-7:00 PM

Room:Concerto A - 3rd Floor

For Part 1 see MS13

The wrinkling or folding of thin sheets is familiar - examples include the coarsening of folds in a hanging drape; the wrinkling of a sheet wrapping a piece of fruit; and the buckling of a compressed thin film. The variety of patterns is great, and we are just beginning to understand how to analyze, simulate, and harness them. This two-part minisymposium highlights the area's interdisciplinary character, combining mathematics with mechanics, experiment with theory, and analysis with computing.

Organizer: Peter Bella
Max Planck Institute for Mathematics in the Sciences, Germany

5:00-5:25 Wrinkles on Curved Surfaces for Aerodynamic Drag Control
Pedro M. Reis, Massachusetts Institute of Technology, USA

5:30-5:55 The Wrinkle Patterns Caused by a Drop on a Sheet
Robert Schroll, Universidad de Santiago de Chile, Chile

6:00-6:25 Plate and Shell Models in Elasticity Obtained by Simultaneous Momogenization and Dimensional Reduction
Igor Velcic, Max Planck Institute for Mathematics in the Sciences, Germany

6:30-6:55 Poking and Wrinkling of Thin Sheets and Shells
Dominic Vella, University of Oxford, United Kingdom

Monday, June 10

MS50

Computational Methods for Nano Scale Materials and Devices - Part I of II

5:00 PM-7:00 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS78

The increasing need for an atomic understanding of many nanoscale materials and devices continues to drive the development of various multiscale modeling and computational methods. The applications include microelectronic and nano-optical device fabrication, semiconductor crystal growth, thin-film engineering, and metal alloy processing, where the nucleation and growth of nano- and microstructures strongly affect the final chemical, electronic, optical and mechanical properties of the materials. The inherent ranges of time and lengths scales in such systems need us to develop reliable methods for linking physical phenomena over multiple scales. This minisymposium will showcase several progresses in developing efficient computational methods towards the aim.

Organizer: Di Liu
Michigan State University, USA

Organizer: Yi Sun
University of South Carolina, USA

5:00-5:25 Multiscale Modeling and Computation of Nano Optical Responses
Di Liu, Michigan State University, USA

5:30-5:55 Dislocation Dynamics in Thin Films Using Fast Multipole Accelerated Boundary Integral Equation Method
Yang Xiang, Hong Kong University of Science and Technology, Hong Kong

6:00-6:25 A Boundary Integral Method for Computing the Dynamics of An Epitaxial Island
Shuwang Li, Illinois Institute of Technology, USA

6:30-6:55 Simulation on Liquid Crystal Elastomers Using Spectral Methods with a New Preconditioner
Wei Zhu, University of Alabama, USA

Monday, June 10

MS51

Phase Field Methods in Materials Science: Recent Developments - Part I of II

5:00 PM-7:00 PM

Room:Rhapsody - 4th Floor

For Part 2 see MS105

Phase field methods have evolved into a useful practical tool as a wide assortment of materials science problems have been addressed using this methodology. As computational power increases, the potential of this methodology is enhanced. Correspondingly, there is also a greater need for modeling and theoretical results. This session will focus on theoretical and computational issues in phase field equations and related methods involving a diffuse interface.

Organizer: Steven M. Wise
University of Tennessee, USA

Organizer: Gunduz Caginalp
University of Pittsburgh, USA

Organizer: Emre Esenturk
Pohang University of Science and Technology, South Korea

5:00-5:25 Some Equations with a Logarithmic Nonlinear Term
Alain Miranville, University of Poitiers, France

5:30-5:55 Nonlocal Phase Field Models
Maurizio Grasselli, Politecnico di Milano, Italy

6:00-6:25 Phase Field Models of Vacancy Mediated Deformation
James Warren, National Institute of Standards and Technology, USA

6:30-6:55 Phase Field Crystal Models with Fast Dynamics
Peter Galenko, University of Jena, Germany

Monday, June 10

MS52

Pattern Formation and Dynamics in Magnetic Materials - Part I of II

5:00 PM-7:00 PM

Room:Minuet - 4th Floor

For Part 2 see MS79

Magnetic materials display a wide range of patterns on a variety of length scales. These patterns can be found as the local minima of a nonlocal and nonconvex variational problem. Their evolution is governed by the Landau-Lifshitz-Gilbert equation, a geometric flow equation leading to additional challenges for analysis and simulations. Recent advances have allowed an understanding of more complex domain patterns and wall structures, and in particular the evolution of these patterns. While slow dynamics have become tractable rigorously, fast timescales are still only accessible numerically.

Organizer: Matthias Kurzke
University of Bonn, Germany

Organizer: Radu Ignat
Universite Paris 11, France

5:00-5:25 Analysis of Complex Domain Patterns in Bulk Ferromagnets
Rudolf Schäfer, Dresden University of Technology, Germany

5:30-5:55 Magnetic Ratchet for 3-dimensional Memory and Logic
Russell P. Cowburn, University of Cambridge, United Kingdom

6:00-6:25 Rotating Vortex-Antivortex Pairs in Ferromagnets under Spin-Polarized Current
Stavros Komineas, University of Crete, Greece

6:30-6:55 The Spin-Cherenkov Effect
Riccardo Hertel, Forschungszentrum Jülich GmbH, Germany; Ming Yan, Shanghai University, China; Attila Kakay, Institute of Solid State Research, Germany

Monday, June 10

MS53

From Microscopic to Continuum: Variational Multiscale Methods: Part II of IV

5:00 PM-7:00 PM

Room:Maestro A - 4th Floor

For Part 1 see MS26
For Part 3 see MS81

This minisymposium addresses new results in the application of variational multiscale methods to systems related to materials science. Different approaches to coupling of the two extreme scales: the microscopic and the continuum will be at the center of the attention. Other recent advances with mesoscopic and multiscale character, such as: homogenization of composite materials, emergence of wrinkling patterns driven by loading or growth, prediction of dislocations and fracture, dimension reduction, microstructures and thin films of nematic liquid crystal, will be discussed. The objective of this minisymposium is to bring together experts and younger scientists from applied mathematics and mechanics to view advances and challenges from different perspectives.

Organizer: Marta Lewicka
University of Pittsburgh, USA

Organizer: Anja Schloemerkemper
University of Würzburg, Germany

5:00-5:25 Lattice Equivalent Models
Annie Raoult, Université Paris Descartes, France; Hervé Le Dret, Université Pierre et Marie Curie, France

5:30-5:55 Variational Analysis of Some Atomistic Systems Exhibiting Spatially-modulated Phases
Marco Cicalese, Technical University of Munich, Germany; Andrea Braides, University of Rome II, Italy

6:00-6:25 Continuum Limit of Microscopic Models of Solids
Jianfeng Lu, New York University, USA

6:30-6:55 Microstructures in Nematic Elastomers
Antonio DeSimone, SISSA/Trieste, Italy

Monday, June 10

Dinner Break

7:00 PM-8:15 PM

Attendeees on their own

PD1

Forward Looking Panel

8:15 PM-9:15 PM

Room:Symphony - 3rd Floor

Chair: Felix Otto, Max Planck Institute for Mathematics in the Sciences, Germany

Chair: Greg Forest, University of North Carolina at Chapel Hill, USA

There is a tradition of this meeting to convene a lively, interactive discussion about Future Directions in the Mathematics of Materials. The primary goal is to give junior scholars a sense of important new directions they might choose to pursue. The panelists are chosen on the basis of their leadership roles in mathematics, science and engineering of materials, important contributions to material science, and their ability to communicate in such a forum. Each panelist will give a short statement, not more than 2 minutes each, followed by a brainstorming session with questions and comments from the audience highly encouraged.

John Brady
California Institute of Technology, USA

Michael Brenner
Harvard University, USA

Maria-Carme Calderer
University of Minnesota, USA

Gero Friesecke
Technische Universität München, Germany

Claude Le Bris
Ecole Nationale des Ponts et Chaussées, France

James Sethian
University of California, Berkeley, USA

Tuesday, June 11

Registration

7:30 AM-5:30 PM

Room:Overture - 3rd Floor

Remarks

8:00 AM-8:15 AM

Room:Symphony - 3rd Floor

IP7

Toward the Principles of Self Assembly and Self Replication

8:15 AM-9:00 AM

Room:Symphony - 3rd Floor

Chair: Greg Forest, University of North Carolina at Chapel Hill, USA

In biological systems, there are striking examples where complicated structures (i.e., the bacterial ribosome) can spontaneously assemble, driven by specific interactions between the components. But how can systems be designed to have this property? Recent technological advances have created the opportunity for making technologically relevant systems that self assemble, by e.g. coating colloidal particles with DNA. We will discuss how self assembly works in this system, through theory, numerical simulation and experiment -- and start to speculate as to whether resulting principles might be useful for unravelling the rules of biological self-assembly. We also outline theoretical constraints on designing this system for self replication.

Michael Brenner
Harvard University, USA

Tuesday, June 11

IP8

Organic Crystal Growth in Thin Films

9:00 AM-9:45 AM

Room:Symphony - 3rd Floor

Chair: Gareth H. McKinley, Massachusetts Institute of Technology, USA

We examine solidification in thin liquid films produced by annealing amorphous films in a solvent vapor. Micrographs captured during annealing reveal the nucleation and growth of single-crystal needles. The needle lengths scale like power laws in time where the growth exponent depends on the thickness of the deposited film. The evolution of the thin film is modeled by a lubrication equation, and an advection-diffusion equation captures the transport of material and solvent within the film. We define a dimensionless transport parameter which describes the relative effects of diffusion and coarsening-driven advection. For large values of this parameter, needle growth matches the theory of 1D, diffusion-driven solidification. For low values, the collapse of droplets -- i.e. coarsening -- drives flow and regulates the growth of needles. Within this regime, we identify and analyze two asymptotic limits: needles that are small compared to the typical drop size, and those that are large.

Anette Hosoi
Massachusetts Institute of Technology, USA

Coffee Break

9:45 AM-10:15 AM

Room:Assembly - 3rd Floor

Tuesday, June 11

MS55

Homogenization and Applications - Part III of III

10:15 AM-12:15 PM

Room:Symphony - 3rd Floor

For Part 2 see MS37

This minisymposium proposal is concerned with recent developments in homogenization and its applications for modeling and understanding the overall response of various types of heterogeneous material systems. The specific topics include nonlinear constitutive behaviors, including finite elasticity and plasticity, as well as coupled properties, including applications to elasto-plastic behavior, ferroelectric and thermoelectric composites, and shape memory polycrystals. In addition, the MS includes presentations dealing with recent advances on universal bounds, instabilities for nematic liquid crystal elastomers, atomistic-to-continuum multi-scale modeling and phononic transport. The 12 presentations are organized in 3 sessions as follows.

Organizer: Pedro Ponte Castaneda
University of Pennsylvania, USA

Organizer: Pierre M. Suquet
CNRS, France

10:15-10:40 Sharp Inequalities which Generalize the Divergence Theorem
Graeme W. Milton, University of Utah, USA

10:45-11:10 Homogenization of Generalized Micro-Resonances and Coupled Properties
Valery Smyshlyaev, University College of London, United Kingdom

11:15-11:40 A Multiscale Atomistic-to-Continuum Method for Atomic Monolayers Undergoing Bending
Kaushik Dayal and Amin Aghaei, Carnegie Mellon University, USA

11:45-12:10 Estimates for Two-phase Nonlinear Conductors via Iterated Homogenization
Martin I. Idiart, Universidad Nacional de La Plata, Argentina; Pedro Ponte Castaneda, University of Pennsylvania, USA

Tuesday, June 11

MS56

The Origins of Hysteresis in Materials - Part I of II

10:15 AM-11:45 PM

Room:Aria B - 3rd Floor

For Part 2 see MS92

Traditionally, hysteresis has been one of the most difficult structure-sensitive properties to predict. In apparently similar materials, processed similarly, the size of the hysteresis loops generated by cycling through a transformation can vary by an order-of-magnitude. Recently, ideas have been put forward by the applied mathematics community that promise to reveal a new understanding of the origins of hysteresis. These ideas have links to fundamental concepts in the calculus of variations of local minimizers, to the analysis of microstructure, and to the mathematical modeling of interfacial energy. The purpose of the minisymposium is to review and compare these timely developments.

Organizer: Richard James
University of Minnesota, USA

Organizer: David Kinderlehrer
Carnegie Mellon University, USA

10:15-10:40 Energy Barriers for Interior Nucleation of Martensite
Hans Knuepfer, University of Bonn, Germany

10:45-11:10 Mathematical Analysis of Microstructures in Low-Hysteresis Shape Memory Alloys: Onset of Complex Patterns
Barbara Zwicknagl, University of Bonn, Germany

11:15-11:40 Hysteresis in Thermodynamically-Consistent Mesoscopic Model of the Ferro/paramagnetic Transition
Martin Kruzik, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Tuesday, June 11

MS57

Multiscale Computation of Fluctuating Hydrodynamics and Microscale Mechanics - Part III of III

10:15 AM-12:15 PM

Room:Aria A - 3rd Floor

For Part 2 see MS30

The hydrodynamics of complex fluids, such as polymer solutions, colloidal suspensions and reactive fluid mixtures, has recently attracted great interest. Coarse-grained models cover a broad range of time and length scales by incrementally sacrificing physical fidelity for computational efficiency. This minisymposium will focus on advances in multiscale numerical methods for simulating flows and biomechanical structures at mesoscopic scales. Issues to be discussed will cover the inclusion of thermal fluctuations in analytical and computational models, coupling of continuum fluids to immersed structures and calibration of effective parameters.

Organizer: Christel Hohenegger
University of Utah, USA

Organizer: Scott McKinley
University of Florida, USA

Organizer: Aleksandar Donev
Courant Institute of Mathematical Sciences, New York University, USA

10:15-10:40 Hybrid Continuum-Particle Thermostats based on Fluctuating Hydrodynamics : Dynamic Implicit-Solvent Coarse-Grained Simulations of Planar Lipid Bilayers and Vesicles
Paul J. Atzberger, University of California, Santa Barbara, USA

10:45-11:10 Regularization Method for the Numerical Solution of Periodic Stokes Flow With Application to Ciliary Beating
Karin Leiderman, University of California, Merced, USA

continued in next column

11:15-11:40 A Computational Model of Microtubule-Based Motion in the Single-Celled C. Elegans Embryo
Tamar Shinar, University of California, Riverside, USA

11:45-12:10 Modeling Neutralization Kinetics of HIV by Broadly Neutralizing Monoclonal Antibodies
Scott McKinley, University of Florida, USA; Alex Chen, SAMSI and UNC at Chapel Hill; Feng B. Shi and Simi Wang, University of North Carolina at Chapel Hill, USA; Peter J. Mucha, University of North Carolina, USA; Greg Forest and Samuel Lai, University of North Carolina at Chapel Hill, USA

Tuesday, June 11

MS58

Metric-driven Deformation of Thin Elastic Sheets - Part III of III

10:15 AM-12:15 PM

Room:Concerto A - 3rd Floor

For Part 2 see MS31

The shape of a thin sheet in R^3 reflects its preference for isometric embedding, and its resistance to bending. When the sheet is Euclidean, isometric embeddings are developable surfaces. But non-Euclidean sheets occur in nature (due to differential growth) and can also be created in the laboratory. We are just beginning to understand how the sheet's metric and its mechanical properties conspire to determine the shape it assumes in space. This 3-part minisymposium highlights the area's interdisciplinary character, combining geometry with analysis, physics with mathematics, and experiment with theory.

Organizer: Robert V. Kohn
Courant Institute of Mathematical Sciences, New York University, USA

10:15-10:40 Metric Description of Discontinuities in Amorphous Elastic Materials
Michael Moshe, The Hebrew University, Israel

10:45-11:10 Monge-Ampère Constraints in Thin Film Elastic Models
Marta Lewicka, University of Pittsburgh, USA; L Mahadevan, Harvard University, USA; *Reza Pakzad*, University of Pittsburgh, USA

11:15-11:40 Growth-Induced Folding, Conformal Maps, and Optimal Design
Chris Santangelo, University of Massachusetts, Amherst, USA

11:45-12:10 Emergence of Spontaneous Twist and Curvature in Non-Euclidean Rods: Application to Erodium Plant Cells
Eran Sharon, The Hebrew University, Israel; Hillel Aharoni, The Hebrew University of Jerusalem, Israel

Tuesday, June 11

MS59

Micro-to-Macro Coarse-Graining and Effective Dynamics in Nonequilibrium Systems - Part III of III

10:15 AM-11:15 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS32

This symposium will bring together speakers who work on Nonequilibrium problems related to materials at various lengthscales ranging from atomic to polycrystalline.

Organizer: Kaushik Dayal
Carnegie Mellon University, USA

10:15-10:40 Covariant Statistical Theory of Phase-Ordering Kinetics via Emergent Symmetries
Stephen J. Watson, University of Glasgow, Scotland, United Kingdom

10:45-11:10 Nonequilibrium Processes for Current Reservoirs
Dimitrios Tsagkarogiannis, University of Crete, Greece; Anna De Masi, Universita di L'Aquila, Italy; Errico Presutti, Universita di Roma "Tor Vergata", Italy; Maria Eulalia Vares, Universidade Federal de Rio de Janeiro, Brazil

Tuesday, June 11

MS60

Dynamic Scaling in Models of Coarsening and Coagulation - Part I of II

10:15 AM-12:15 PM

Room:Rhapsody - 4th Floor

For Part 2 see MS87

Coarsening phenomena and cluster formation appear in many areas of materials science such as grain growth in polycrystalline materials, phase separation in alloys or dewetting of thin polymer films. Experiments often suggest that typical length scales in such systems follow universal scaling laws. A variety of mathematical models have been proposed over the last century to describe these systems, ranging from discrete and continuous mean-field type models to Cahn-Hilliard equations. A rigorous mathematical justification of scaling laws is however largely lacking and remains a major challenge. The speakers in this minisymposium will discuss new heuristic, analytical and numerical techniques to derive dynamic scaling laws in a variety of models.

Organizer: Barbara Niethammer
University of Bonn, Germany

Organizer: Joseph Conlon
University of Michigan, USA

10:15-10:40 Coarsening for the Diffusive Carr-Penrose Model
Joseph Conlon and Jingchen Wu, University of Michigan, USA

10:45-11:10 Motion of Interfaces Under the Cahn-Hilliard Equation with One or Two Sided Degenerate Diffusion Mobility
Shibin Dai, Michigan State University, USA; Qiang Du, Pennsylvania State University, USA

11:15-11:40 Self-similar Solutions to Coagulation Equations
Juan Velazquez, University of Bonn, Germany

11:45-12:10 Exponential Convergence to Equilibrium for Subcritical Solutions of the Becker-Döring Equations
Jose A. Cañizo, University of Birmingham, United Kingdom; Bertrand Lods, Università degli Studi di Torino, Italy

Tuesday, June 11

MS61

The Ginzburg-Landau Model and Related Topics - Part III of V

10:15 AM-11:45 AM

Room:Minuet - 4th Floor

For Part 2 see MS34
For Part 2 see MS88

The focus of the minisymposium is on mathematical problems related to Ginzburg-Landau model with application in physics and materials science including but not limited to: superconductivity, superfluidity, liquid crystals, and polymers. The speakers in this minisymposium will describe their recent research including the development and structure of singular solutions of the Ginzburg-Landau-type problems and the dynamics of vortex motion.

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Yaniv Almog
Louisiana State University, USA

Organizer: Leonid Berlyand
Pennsylvania State University, USA

10:15-10:40 Navigating Energy Landscapes in Ginzburg-Landau Problems with Long-Range Interactions
Rustum Choksi, McGill University, Canada

10:45-11:10 Front Propagation in Stratified Media: A Variational Approach
Cyrill B. Muratov, New Jersey Institute of Technology, USA; Matteo Novaga, University of Padova, Italy

11:15-11:40 Projection Valued Functions on Perforated Domains in the Plane
Alberto Montero, Pontificia Universidad Católica de Chile, Chile; Dmitry Golovaty, University of Akron, USA

Tuesday, June 11

MS62

Electronic Structure - Part III of IV

10:15 AM-12:15 PM

Room:Maestro A - 4th Floor

For Part 2 see MS35
For Part 4 see MS89

Predicting the elctronic structure of complex molecular and condensed-matter systems has been a focus of attention in chemistry and physics for decades. More recently, espceically since the advent of density functional theory (DFT), it has also become an important ingredient in materials science. Electronic structure models allows the on-the-fly computation of non-empirical and chemically specific interatomic interactions within larger-scale simulations.

Organizer: Gero Friesecke
Technische Universität München, Germany

Organizer: Eric Cances
Ecole des Ponts and INRIA, France

Organizer: Lin Lin
Lawrence Berkeley National Laboratory, USA

Organizer: Chao Yang
Lawrence Berkeley National Laboratory, USA

10:15-10:40 Efficient Algorithms for (Di-)Atomic Basis Sets
Christian B. Mendl, Technische Universität München, Germany

10:45-11:10 Higher-order Adaptive Finite-element Methods for Large-scale Electronic Structure Calculations using Kohn-Sham Density Functional Theory
Phani S. Motamarri and Vikram Gavini, University of Michigan, USA

11:15-11:40 Finite Elements for Large-Scale Electronic Structure Calculations: From Classical to Enriched to Discontinuous
John Pask, Lawrence Livermore National Laboratory, USA

11:45-12:10 Entanglement Based Algortihms for Electronic Structure Computation of Strongly Correlated Systems
Reinhold Schneider, Technische Universität Berlin, Germany

Tuesday, June 11

MS63

Nonlinear Lattice Dynamics - Part III of III

10:15 AM-12:15 PM

Room:Maestro B - 4th Floor

For Part 2 see MS45

Many problems in materials science concern phenomena where an interplay between discreteness and dynamics plays a fundamental role. Examples include propagation of defects, pattern formation and emergence of complexity and the application range from metamaterials to granular media. The main mathematical issues concern interaction between nonlinearity and dispersion, extremely ragged energy landscapes, trapping, depinning and radiative damping. This minisymposium features talks by leading experts in nonlinear lattice dynamics and aims at facilitating the exchange of ideas and at highlighting the most important unsolved problems in this field.

Organizer: Anna Vainchtein
University of Pittsburgh, USA

Organizer: Lev Truskinovsky
Ecole Polytechnique, France

10:15-10:40 Travelling Waves in the Discrete FitzHugh-Nagumo Model
Hermen Jan Hupkes, University of Leiden, The Netherlands; *Bjorn Sandstede*, Brown University, USA

10:45-11:10 Macroscopic Interface Dynamics in Forward-backward Lattice Diffusion
Michael Helmers, University of Bonn, Germany; Michael Herrmann, Saarland University, Germany

11:15-11:40 Mesoscopic Peridynamics Derived from Microstructure
Alexander Panchenko, Washington State University, USA

11:45-12:10 Solitary Waves in the FPU Chain: A New Exact Solution
Anna Vainchtein, University of Pittsburgh, USA; Lev Truskinovsky, Ecole Polytechnique, France

Lunch Break

12:15 PM-1:30 PM

Attendees on their own

Tuesday, June 11

IP9

Metamaterials: High Contrast Composites with Unusual Properties

1:30 PM-2:15 PM

Room:Symphony - 3rd Floor

Chair: Robert P. Lipton, Louisiana State University, USA

Composite materials can have properties unlike any found in nature, and in this case they are known as metamaterials. Materials with negative Poisson's ratio or negative refractive index are now classic examples. The effective mass density, which governs the propogation of elastic waves in a metamaterial can be anisotropic, negative, or even complex. Even the eigenvectors of the effective mass density tensor can vary with frequency. One of the exciting applications of metamaterials is to cloaking, yet we show here that there are limitations to electromagnetic cloaking: one cannot get broadband passive cloaking if the surrounding material is air, at least in the quasistatic limit. Non-linear metamaterials are also interesting and a basic question is what non-linear behaviors can one get in periodic materials constructed from rigid bars and pivots? It turns out that the range is enormous. Materials for which the only easy mode of macroscopic deformation is an affine deformation, can be classed as unimode, bimode, trimode,...hexamode, acccording to the number of easy modes of deformation. We give a complete chacterization of possible behaviors of nonlinear unimode materials.

Graeme W. Milton
University of Utah, USA

Intermission

2:15 PM-2:30 PM

Tuesday, June 11

MS64

Mathematical and Computational Aspects of Peridynamics and Related Nonlocal Models - Part I of IV

2:30 PM-4:30 PM

Room:Symphony - 3rd Floor

For Part 2 see MS73

Nonlocal models have been proposed in the past years to overcome limitations presented in local classical models. In particular, "strong" nonlocal models involving integro-differential equations, with integrands based upon differences of field quantities, provide an alternative framework to local models based upon partial differential equations. Models of this kind include peridynamics for solid mechanics and nonlocal diffusion, among others. Their novelty, however, introduces challenges from the mathematical and computational perspectives, including characterization of solutions, discretization schemes, modeling of engineering systems, description of coupled models, validation, verification, and uncertainty quantification, etc. This minisymposium invites contributions on recent developments in peridynamics and related nonlocal models.

Organizer: Pablo Seleson
University of Texas at Austin, USA

Organizer: Qiang Du
Pennsylvania State University, USA

Organizer: Michael L. Parks
Sandia National Laboratories, USA

2:30-2:55 Peridynamic Balance Laws
Richard B. Lehoucq, Sandia National Laboratories, USA

3:00-3:25 Peridynamic Instability and Damage
Robert P. Lipton, Louisiana State University, USA

continued in next column

3:30-3:55 Calibration and Ranking of Stochastic Peridynamics Models for Ring Fragmentation Phenomena
Ernesto E. Prudencio, University of Texas at Austin, USA; Michael L. Parks, Sandia National Laboratories, USA

4:00-4:25 Intersonic Crack Propagation in Fiber-Reinforced Composites: a Peridynamic Approach
Florin Bobaru, University of Nebraska, Lincoln, USA; Yenan Wang, University of Nebraska-Lincoln, USA

Tuesday, June 11

MS65

Geometrical Instabilities in Soft Materials - Part I of II

2:30 PM-4:30 PM

Room:Aria B - 3rd Floor

For Part 2 see MS102

The macroscopic properties and failure mechanisms of a truly diverse variety of solids are known to be the eventual manifestation of instabilities that occur across a broad range of length scales. This symposium will address recent advances in the mathematical modeling of such local instabilities. Topics of particular interest include: i) Cavitation and fracture; ii) Creasing and wrinkling; iii) Microstructural instabilities in heterogeneous material systems responsive to coupled stimuli such as electrostrictive and liquid crystal elastomers.

Organizer: Oscar Lopez-Pamies
University of Illinois at Urbana-Champaign, USA

Organizer: Scott Spector
Southern Illinois University, USA

2:30-2:55 Austenite As a Local Minimizer in a Model of Material Microstructure with a Surface Energy Term

Jonathan J. Bevan, University of Surrey, United Kingdom

3:00-3:25 Swell Induced Wrinkling and Creasing on the Surface of Hydrogel Bilayers

Nikolaos Bouklas, University of Texas at Austin, USA; Zhigen Wu, Hefei University of Technology, China; *Rui Huang*, University of Texas at Austin, USA

3:30-3:55 Stability Conditions for Constrained and Unconstrained Multi-Phase Elastic Solids

Dennis M. Kochmann and Charles Wojnar, California Institute of Technology, USA

4:00-4:25 Thermal Shock Crack Initiation: a Non Local Damage Model Stability Analysis

Jean-Jacques Marigo, Université Pierre et Marie Curie, France; *Paul Sicsic*, École Polytechnique, France

Tuesday, June 11

MS66

Motility and Mechanics of Biomolecular Complexes - Part II of III

2:30 PM-4:30 PM

Room:Aria A - 3rd Floor

For Part 1 see MS39
For Part 3 see MS84

This symposium will focus on problems which draw on ideas from solid, fluid and statistical mechanics. Problems in soft materials, elastomers and biophysics are already of this nature. But, we anticipate that areas such as, complex fluids, mechanics of self-propulsion, etc., where there is significant overlap with chemistry can also benefit from mathematical approaches where Brownian motion is accounted for. Some representative topics in this symposium include: (a) Fluctuating rod models for biopolymers, (b) Mechanics of force generation in cells, (c) Swimming and self-propulsion in complex fluids, (d) Coarse-grained simulations of cellular organelles, (e) Phase transitions in macromolecular complexes.

Organizer: Prashant K. Purohit
University of Pennsylvania, USA

Organizer: Antonio De Simone
SISSA, Italy

2:30-2:55 Cytoskeletal Mechanics and Cell Motility

Antonio DeSimone, SISSA/Trieste, Italy

3:00-3:25 Lamellipodia Dynamics in Motile Cells

Sefi Givli, Technion, Israel; Yair Adler, Technion Israel Institute of Technology, Israel

3:30-3:55 Swimming Micro-organisms in Complex Fluids

Thomas R. Powers, Brown University, USA

4:00-4:25 Cellular Pressure and Volume Regulation and Implications for Cell Mechanics and Cell Motility

Sean Sun, Johns Hopkins University, USA

Tuesday, June 11

MS67

Mathematical Modeling of Dislocations in Crystalline Solids - Part I of II

2:30 PM-4:30 PM

Room:Concerto A - 3rd Floor

For Part 2 see MS103

The focus of the minisymposium will be on mathematical issues in studies of dislocations - defects in a crystalline lattice structure that play an important role in defining macroscopic properties of solids. The speakers will discuss their recent results in modeling of dislocations at all levels - from microscopic to macroscopic - and on exploring connections between various length- and timescales.

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Malena I. Espanol
University of Akron, USA

2:30-2:55 Strain and Rotation Fields of Dislocations in Graphene

Luis Bonilla, Universidad Carlos III de Madrid, Spain; Ana Carpio, Universidad de Complutense de Madrid, Spain; Jamie Warner, University of Oxford, United Kingdom

3:00-3:25 Pattern Formation in Indentation Tests

Ana Carpio, Universidad Complutense de Madrid, Spain

3:30-3:55 Plastic Strain Recovery in Nanocrystalline Nickel

Marisol Koslowski and Yuesong Xie, Purdue University, USA

4:00-4:25 Kinematic Analysis of Finite Plasticity as the Limit of Dislocation Activity

Celia Reina Romo, California Institute of Technology, USA; Sergio Conti, University of Duisburg-Essen, Germany

Tuesday, June 11

MS68

Stochastic Methods in Molecular Simulation: Theory and Applications - Part I of II

2:30 PM-4:30 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS86

Molecular modeling and simulation relies crucially on stochastic models, from the most theoretical aspects (e.g. the justification of transition state theory, and associated Markov jump models), to the most standard simulation codes where Monte-Carlo methods are used. The goal of the minisymposium is to bring together both theoreticians (in applied mathematics and/or theoretical physics) and scientists involved in practical numerical simulations, so that they can share their different point of views.

Organizer: Mathias Rousset
INRIA Rocquencourt, France

Organizer: Tony Lelievre
CERMICS ENPC, France

2:30-2:55 Using Coarse Grained Models to Speed Convergence to the Minimum Energy Pathway
Jonathan Weare, Bo Qi, Seyit Kale, and Aaron Dinner, University of Chicago, USA

3:00-3:25 Local Hyperdynamics
Arthur F. Voter, Los Alamos National Laboratory, USA

3:30-3:55 Long-Time Simulation of Steady Nonequilibrium Flow
Matthew Dobson, CERMICS ENPC, France

4:00-4:25 Markov Model Reduction with Perturbed Test Functions
Mathias Rousset, INRIA Rocquencourt, France

Tuesday, June 11

MS69

Recent Developments in Modeling Crystallization and Material Properties with Periodic Fields - Part III of III

2:30 PM-4:30 PM

Room:Rhapsody - 4th Floor

For Part 2 see MS33

Employing free energy functionals that are minimized by periodic fields allows one to study a variety of phenomena including nucleation and growth, epitaxial growth, yield strength of polycrystals, grain boundary melting and glass formation. This approach is the basis of dynamical classical density functional theory and phase field crystal models. There has been tremendous activity in this field including applications in liquid crystals, ordering on curved surfaces and hydrodynamic/crystal interaction. This minisymposium will explore recent advances in three major avenues namely specific applications in material science, extensions to more complex systems and the connection between various approaches and traditional methods.

Organizer: Arvind Baskaran
University of California, Irvine, USA

Organizer: Ken Elder
Oakland University, USA

Organizer: John Lowengrub
University of California, Irvine, USA

2:30-2:55 Modeling Multiferroic Polycrystalline Materials
Ken Elder, Oakland University, USA

3:00-3:25 Two-Dimensional Crystals - the Interplay of Geometry and Materials Defects
Axel Voigt, Technische Universität Dresden, Germany

continued in next column

3:30-3:55 Fluctuating Nonlinear Hydrodynamics formalism of the Density Functional Theory of solidification.
Gyula Toth and György Tegze, Wignes Research Centre for Physics, Hungary; Laszlo Granasy, Research Institute for Solid State Physics & Optics, Budapest, Hungary

4:00-4:25 Phase Field Crystals - Modeling Structural Transformations at Diffusive Time Scales and Atomic Length Scales
Michael Greenwood, Natural Resources Canada

Tuesday, June 11

MS70

Modeling and Computations of Liquid Crystal Polymers and Active Nematic Suspensions - Part II of II

2:30 PM-4:30 PM

Room:Minuet - 4th Floor

For Part 1 see MS25

Liquid crystal polymers and active nematic suspensions have attracted much attention in the past because of their wide applications in many environmental and industrial applications. Due to the nonlinear coupling of various complex physical phenomena, their modeling, analysis and numerical simulations are remarkably challenging. The main purpose of this minisymposium is to present some new developments and enhance collaborations in these areas.

Organizer: Ruhai Zhou
Old Dominion University, USA

Organizer: Qi Wang
University of South Carolina, USA

Organizer: Xiaofeng Yang
University of South Carolina, USA

2:30-2:55 Application of Active Liquid Crystal Models to Complex Biological Systems
Qi Wang, University of South Carolina, USA

3:00-3:25 Kinetic Theory and Simulations of Active Nematic Polymers
Ruhai Zhou, Old Dominion University, USA; M. Gregory Forest, University of North Carolina at Chapel Hill, USA; Qi Wang, University of South Carolina, USA

3:30-3:55 Chiral Liquid Crystals in Poiseuille Flow
Zhenlu Cui, Fayetteville State University, USA

4:00-4:25 Modeling and Simulation of Organic Superconductors
H.Q. Lin, The Chinese University of Hong Kong, Hong Kong

Tuesday, June 11

MS71

Geometric Variational Problems with Long-range Interactions - Part I of II

2:30 PM-4:30 PM

Room:Maestro A - 4th Floor

For Part 2 see MS106

Variational problems involving competing short-range and long-range interactions often arise in the studies of phase transitions in different materials and, more broadly, in systems exhibiting energy driven pattern formation. In the recent few years, there has been much work on two basic paradigms: The Ohta-Kawasaki energy functional, which arises as a model of self-assembly in diblock copolymer melts, and isoperimetric problems in the presence of long-range forces. This minisymposium will focus on recent analytical advances in these and related problems, with a focus on geometric properties on energy minimizing interfaces. Extensions to diffuse interface models and related problems will also be explored.

Organizer: Rustum Choksi
McGill University, Canada

Organizer: Cyrill B. Muratov
New Jersey Institute of Technology, USA

2:30-2:55 Existence and Qualitative Properties of Grounds States to the Non-Local Choquard-Type Equations
Vitaly Moroz, Swansea University of South Wales, United Kingdom

3:00-3:25 Nonexistence Results for Energy Functionals with Competing Attracting and Repelling Interactions
Jianfeng Lu, New York University, USA

3:30-3:55 Minimization of a Short-range Attractive and Long-range Repulsive Energy Related to a Nonlocal Aggregation Model
Ihsan A. Topaloglu, McGill University, Canada

4:00-4:25 Verifying Global Minimizers for Ginzburg-Landau-type Problems: a Simple Approach via Convex Approximation
David Shirokoff, McGill University, Canada

Tuesday, June 11

MS72

Morphological Evolution of Crystalline Surfaces, Thin Films, and Clusters - Part I of II

2:30 PM-4:30 PM

Room:Maestro B - 4th Floor

For Part 2 see MS99

Non-equilibrium morphological evolution of crystalline surfaces and thin films, and of supported or liquid-phase clusters, is a key element of nanotechnology. Despite some progress, many related phenomena remain poorly understood. A central issue is to reconcile descriptions across several time and length scales, from atomistic to mesoscale to continuum. Unresolved problems include far-from-equilibrium growth shapes during self-assembly of clusters by surface deposition or in liquid-phase synthesis, multilayer growth and faceting, stochastic fluctuations of surface features, and post-growth relaxation and stability of nanostructures. This minisymposium reviews recent advances in modeling, analysis and simulation.

Organizer: Dionisios Margetis
University of Maryland, College Park, USA

Organizer: Jim W. Evans
Iowa State University, USA

2:30-2:55 Nanocluster Self-assembly: Far-from-equilibrium Shapes and Composition Profiles
Jim W. Evans, Iowa State University, USA

3:00-3:25 Kinetics in GaAs Thin-Film Growth with First-Principles Local Superbasin Kinetic Monte Carlo
Kristen Fichthorn, Pennsylvania State University, USA

continued on next page

3:30-3:55 Directed Assembly of Nanoclusters on a Templated Surface: Rumpled Graphene
Yong Han, Iowa State University, USA

4:00-4:25 Analyzing Capture Zone Distributions (CVDs) in Growth: Theory and Applications
Theodore L. Einstein, University of Maryland, USA; Alberto Pimpinelli, Rice University, USA; DiegoLuis González, Universidad del Valle, Cali, Colombia; Rajesh Sathiyanarayanan, IBM Semiconductor Research & Development, Bangalore, India; Ajmi Hammouda, University of Monastir, Tunisia

Coffee Break

4:30 PM-5:00 PM

Room:Assembly - 3rd Floor

Tuesday, June 11

MS73

Mathematical and Computational Aspects of Peridynamics and Related Nonlocal Models - Part II of IV

5:00 PM-7:00 PM

Room:Symphony - 3rd Floor

For Part 1 see MS64
For Part 3 see MS82

Nonlocal models have been proposed in the past years to overcome limitations presented in local classical models. In particular, "strong" nonlocal models involving integro-differential equations, with integrands based upon differences of field quantities, provide an alternative framework to local models based upon partial differential equations. Models of this kind include peridynamics for solid mechanics and nonlocal diffusion, among others. Their novelty, however, introduces challenges from the mathematical and computational perspectives, including characterization of solutions, discretization schemes, modeling of engineering systems, description of coupled models, validation, verification, and uncertainty quantification, etc. This minisymposium invites contributions on recent developments in peridynamics and related nonlocal models.

Organizer: Pablo Seleson
University of Texas at Austin, USA

Organizer: Qiang Du
Pennsylvania State University, USA

Organizer: Michael L. Parks
Sandia National Laboratories, USA

5:00-5:25 Mathematical and Numerical Analysis of Nonlocal Models
Qiang Du, Pennsylvania State University, USA

continued in next column

5:30-5:55 Conditioning in Fractional Sobolev Spaces
Burak Aksoylu and Zuhal Unlu, Louisiana State University, USA

6:00-6:25 Variational Analysis of Linearized Peridynamics for Heterogeneous Materials
Tadele Mengesha, Louisiana State University, USA

6:30-6:55 Sparse Dynamics of Non-Local Evolution Equations
Hayden Schaeffer, Stanley J. Osher, and Russel Caflisch, University of California, Los Angeles, USA; Cory Hauck, Oak Ridge National Laboratory, USA

Tuesday, June 11

MS74

Methods and Applications in the Optimization of Materials Composition - Part II of II

5:00 PM-7:00 PM

Room:Aria B - 3rd Floor

For Part 1 see MS11

The fundamental variables in materials design are the materials' compositions. Due to the essentially infinite space of possible materials, it is necessary to develop efficient methods for optimizing properties of materials. Compositional materials design is a mixed discrete and continuous optimization problem since each composition may support several stable arrangements of its constituent elements leading to complex and high-dimensional surfaces. Current development efforts run from deterministic branch-and-bound or (local) gradient-based methods to (global) stochastic algorithms, with and without constraints. The symposium will cover recent advances in the development and application of optimization algorithms to the materials design problem.

Organizer: Berend C. Rinderspacher
Army Research Laboratory, USA

5:00-5:25 Rational Design of Molecular Materials: Piezoelectrics and Organic Solar Cells Via Genetic Lgorithms
Geoffrey Hutchison, University of Pittsburgh, USA

5:30-5:55 Data Mining Big Materials Data
Shyue Ping Ong, Massachusetts Institute of Technology, USA

continued in next column

6:00-6:25 Numerical Algorithms for Identification of Optimal Parameters in Material Models for Industrial Forming Processes
Marco Rozgic, Helmut-Schmidt-Universitaet Hamburg, Germany; Yalin Kiliclar, Ivaylo Vladimirov, and Stefanie Reese, RWTH Aachen University, Germany; Marcus Stiemer, Helmut-Schmidt-University of Federal Armed Forces Hamburg, Germany

6:30-6:55 Taking Advantage of the Convexity of Chemical Compund Space
Berend C. Rinderspacher, Army Research Laboratory, USA

Tuesday, June 11

MS75

Active Fluids and Living Liquid Crystals - Part I of II

5:00 PM-7:00 PM

Room:Aria A - 3rd Floor

For Part 2 see MS93

Active fluids are an exciting class of complex fluids in which particles individually consume energy and collectively generate coherent translational or rotational motion. In many of these systems the individual particles can form orientational order, hence the name of living liquid crystals. The novel type of non-equilibrium dynamics makes theoretical modeling and experimental exploration of such systems extremely challenging. The goal of this symposium is to bring together a group of theorists and experimentalists from different disciplines to share the most recent results in this field, and enhance collaborations to tackle open questions in the study of such complex fluids.

Organizer: M. Cristina Marchetti, *Syracuse University, USA*

Organizer: Zhenlu Cui
Fayetteville State University, USA

Organizer: Peter Palffy-Muhoray
Kent State University, USA

5:00-5:25 Spontaneous Flow in Active Gels
Tim Sanchez, Brandeis University, USA

5:30-5:55 Excitability and Chaos in Active Nematic Suspensions
Luca Giomi, SISSA, Trieste, Italy

6:00-6:25 The Metaphase Spindle As An Active Liquid Crystal
Dan Needleman, Harvard University, USA

6:30-6:55 Dynamical Structures in Active Nematics and Their Novel Behaviors
Xia-qing Shi, Soochow University, China

Tuesday, June 11

MS76

Multiscale Study of Defects in Solids - Part I of III

5:00 PM-7:00 PM

Room:Concerto A - 3rd Floor

For Part 2 see MS85

The structures of lattice defects in solids are often responsible for many observed macroscale material properties. A full understanding of the role of defect structures typically requires a multiscale approach. This minisymposium will focus on the mathematical analysis of defect properties, accurate and robust computer simulation methods, coupled atomistic and continuum models, and coarse-graining approaches from atomistic to mesoscpoic and continuum description.

Organizer: Xiantao Li
Pennsylvania State University, USA

Organizer: Yang Xiang
Hong Kong University of Science and Technology, Hong Kong

Organizer: Zhijian Yang
Wuhan University, China

5:00-5:25 Continuum Models for Dislocation Dynamics and Crystal Plasticity
Yang Xiang and Yichao Zhu, Hong Kong University of Science and Technology, Hong Kong

5:30-5:55 Continuum Limit of Discrete Motion of Interfaces
Andrea Braides, University of Rome, Italy; Marco Cicalese, Technical University of Munich, Germany; *Aaron Yip*, Purdue University, USA

6:00-6:25 From Atomistic to Continuum Boundary Value Problems in Nonlinear Elasticity
Bernd Schmidt, Augsburg College, USA

6:30-6:55 Reformulation of Continuum Mechanics for Multiscale Simulation
Youping Chen, University of Florida, USA

Tuesday, June 11

MS77

Computational Tools for Metastable Systems - Part III of III

5:00 PM-7:00 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS41

Many materials, including crystals, metals and biological media, possess metastable states that introduce a severe time scale separation. Consequently, direct numerical simulations may be unable to observe important transitions, such as the migration of a defect through a crystal or the folding of a protein. A variety of techniques have been proposed to accelerate these computations, including accelerated dynamics and kinetic Monte Carlo. In this minisymposium, we present recent advances and analysis of such techniques.

Organizer: Gideon Simpson
University of Minnesota, USA

Organizer: Jonathan Weare
University of Chicago, USA

Organizer: Arthur F. Voter
Los Alamos National Laboratory, USA

Organizer: Mitchell Luskin
University of Minnesota, USA

5:00-5:25 Multiscale Modeling of Macromolecular Dynamics
Cecilia Clementi, Rice University, USA

5:30-5:55 An Infinite Swapping Approach to the Rare-Event Sampling Problem
Nuria Plattner, Freie Universitaet Berlin, Germany

6:00-6:25 Recent Developments in Adaptive Kinetic Monte Carlo
Graeme Henkelman and *Samuel Chill*, The University of Texas at Austin, USA

6:30-6:55 Wang-Landau Multiple State Transition Interface Sampling
Peter Bolhuis, University of Amsterdam, Netherlands

Tuesday, June 11

MS78

Computational Methods for Nano Scale Materials and Devices - Part II of II

5:00 PM-7:00 PM

Room:Rhapsody - 4th Floor

For Part 1 see MS50

The increasing need for an atomic understanding of many nanoscale materials and devices continues to drive the development of various multiscale modeling and computational methods. The applications include microelectronic and nano-optical device fabrication, semiconductor crystal growth, thin-film engineering, and metal alloy processing, where the nucleation and growth of nano- and microstructures strongly affect the final chemical, electronic, optical and mechanical properties of the materials. The inherent ranges of time and lengths scales in such systems need us to develop reliable methods for linking physical phenomena over multiple scales. This minisymposium will showcase several progresses in developing efficient computational methods towards the aim.

Organizer: Di Liu
Michigan State University, USA

Organizer: Yi Sun
University of South Carolina, USA

5:00-5:25 Localized Bases for Numerical Homogenization of Heterogeneous Materials
Lei Zhang, Shanghai Jiao Tong University, China

5:30-5:55 A Hierarchy of Coarse-Grained Molecular Dynamics Models for Material Defects
Xiantao Li, Pennsylvania State University, USA

6:00-6:25 Fast Nanowire Simulations Using a Hash Table-Based Cache
Kris Reyes, University of Michigan, USA

6:30-6:55 Kinetic Monte Carlo Simulations of Multicellular Aggregate Self-Assembly in Biofabrication
Yi Sun, University of South Carolina, USA

Tuesday, June 11

MS79

Pattern Formation and Dynamics in Magnetic Materials - Part II of II

5:00 PM-7:00 PM

Room:Minuet - 4th Floor

For Part 1 see MS52

Magnetic materials display a wide range of patterns on a variety of length scales. These patterns can be found as the local minima of a nonlocal and nonconvex variational problem. Their evolution is governed by the Landau-Lifshitz-Gilbert equation, a geometric flow equation leading to additional challenges for analysis and simulations. Recent advances have allowed an understanding of more complex domain patterns and wall structures, and in particular the evolution of these patterns. While slow dynamics have become tractable rigorously, fast timescales are still only accessible numerically.

Organizer: Matthias Kurzke
University of Bonn, Germany

Organizer: Radu Ignat
Universite Paris 11, France

5:00-5:25 The Cross-over from Symmetric to Asymmetric Domain Walls in Soft Ferromagnetic Films
Lukas Döring, Max Planck Institute for Mathematics in the Sciences, Germany; Radu Ignat, Universite Paris 11, France; Felix Otto, Max Planck Institute for Mathematics in the Sciences, Germany

5:30-5:55 Ferromagnetism Modeling: from Micro-Scale to Meso-Scale
Stéphane Labbé, Université de Grenoble I, France

6:00-6:25 Domain Wall Motion in Ferromagnetic Nanowires
Valeriy Slastikov and Jonathan Robbins, University of Bristol, United Kingdom; Arseni Goussev, Northumbria University, United Kingdom

6:30-6:55 Boundary Vortices in Micromagnetics
Radu Ignat, Universite Paris 11, France; Matthias Kurzke, University of Bonn, Germany

Tuesday, June 11

MS80

Advances in Modeling and Computation of Thin Liquid Films in Materials Science - Part I of II

5:00 PM-7:00 PM

Room:Maestro A - 4th Floor

For Part 2 see MS98

We propose a two-session minisymposium focusing on modeling and numerical simulation of thin films. This minisymposium will bring together mathematicians, physicists, and engineers at the frontier of the research in thin liquid films in materials science. The two-session minisymposium will allow vibrant and timely discussion and rich exchange of ideas. Topics will include: new computational and analytical methods for modeling interfaces and contact lines, coupling between atomic level and continuum simulations, self and directed assembly, liquid-crystal statics and dynamics, and applications to micro- and nano-fluidics. Speakers will include distinguished international experts including experimental researchers, as well as junior and early-career researchers with expertise in thin films.

Organizer: Shahriar Afkhami
New Jersey Institute of Technology, USA

Organizer: Linda Cummings
New Jersey Institute of Technology, USA

Organizer: Lou Kondic
New Jersey Institute of Technology, USA

5:00-5:25 Theoretical Modeling of Droplet Breakup and Generation in Microfluidic Devices
Alexander M. Leshansky, Technion IIT, Haifa, Israel

continued in next column

5:30-5:55 Assembly of Anisotropic Particles at Interfaces
Kathleen Stebe, University of Pennsylvania, USA

6:00-6:25 Numerical Simulation of Dewetting of Nanodroplets
Shahriar Afkhami, New Jersey Institute of Technology, USA

6:30-6:55 Self-Similar Rupture in Marangoni-Driven Thin Fluid Sheets
Burt S. Tilley, Worcester Polytechnic Institute, USA

Tuesday, June 11

MS81

From Microscopic to Continuum: Variational Multiscale Methods: Part III of IV

5:00 PM-7:00 PM

Room:Maestro B - 4th Floor

For Part 2 see MS53
For Part 2 see MS107

This minisymposium addresses new results in the application of variational multiscale methods to systems related to materials science. Different approaches to coupling of the two extreme scales: the microscopic and the continuum will be at the center of the attention. Other recent advances with mesoscopic and multiscale character, such as: homogenization of composite materials, emergence of wrinkling patterns driven by loading or growth, prediction of dislocations and fracture, dimension reduction, microstructures and thin films of nematic liquid crystal, will be discussed. The objective of this minisymposium is to bring together experts and younger scientists from applied mathematics and mechanics to view advances and challenges from different perspectives.

Organizer: Marta Lewicka
University of Pittsburgh, USA

Organizer: Anja Schloemerkemper
University of Würzburg, Germany

5:00-5:25 Asymptotic Analysis of Prestrained Materials
Marta Lewicka, University of Pittsburgh, USA

5:30-5:55 Local and Non-Local Continuum Limits of Energies for Spin Systems
Roberto Alicandro, Università di Cassino, Italy; Nadia Ansini, Unaffiliated; Maria Stella Gelli, Universita' di Pisa, Italy

continued in next column

6:00-6:25 Atomistic Energy Minimization and Wulff Shapes
Gero Friesecke, Technische Universität München, Germany

6:30-6:55 A Discrete-to-Continuum Model for Thin Rods Made from a Biphase Material
Giuliano Lazzaroni, University of Würzburg, Germany; Mariapia Palombaro, University of L'Aquila, Italy; Anja Schlömerkemper, University of Würzburg, Germany

Dinner Break

7:00 PM-8:15 PM

Attendees on their own

SIAG/MS Business Meeting

8:15 PM-9:00 PM

Room:Symphony - 3rd Floor

Complimentary wine and beer will be served.

Wednesday, June 12

Registration

7:30 AM-5:30 PM

Room:Overture - 3rd Floor

Closing Remarks

8:00 AM-8:15 AM

Room:Symphony - 3rd Floor

IP10

The Dynamics of Liquid Crystals

8:15 AM-9:00 AM

Room:Symphony - 3rd Floor

Chair: Patricia Bauman, Purdue University, USA

Many of the beautiful results of solid state physics are predicated on the positional order of the constituents of solid crystals. Liquid crystals are soft materials, characterized by orientational order whose implications and consequences are less well understood. Emerging new materials bring diversity to the symmetry, composition, length- and time-scales and interactions of orientationally ordered soft matter systems. The salient feature of these systems is their symmetry-mandated responsivity to stimuli. In this talk, I will describe dynamic phenomena in a variety of liquid crystalline systems in response to different excitations, and discuss approaches and challenges to modeling the dynamic response.

Peter Palffy-Muhoray
Kent State University, USA

Wednesday, June 12

IP11

Multiscale Mathematics and Renewable Energy

9:00 AM-9:45 AM

Room:Symphony - 3rd Floor

Chair: Greg Forest, University of North Carolina at Chapel Hill, USA

It is well understood that access to cheap energy underpins modern societies and that there is a direct correlation between a nation's energy consumption per capita and its GDP. Finding enough energy to fuel industrialized economies and pull developing countries out of poverty without overheating the climate is a central challenge of the 21st century. Meeting it will require new technologies for producing, storing, and using energy with performance levels far beyond what is currently possible. Such technologies spring from scientific breakthroughs in new materials and chemical processes that govern the transfer of energy between light, electricity and chemical fuels. In applications ranging from renewable fuels production to generating electricity from wind and solar through energy storage, advanced materials play a crucial role in accelerating the development of new energy solutions. In this talk we will discuss mathematical approaches to modeling required to address the complexities of renewable energy technologies, which include coupled physical, chemical and biological processes, broad spans of spatial and temporal scales, many sources of uncertainty, and, in some instances, only a primitive understanding of the fundamental processes and phenomena.

Steven Hammond
National Renewable Energy Laboratory, USA

Coffee Break

9:45 AM-10:15 AM

Room:Assembly - 3rd Floor

Wednesday, June 12

MS27

Mathematical Methods for Epitaxial Growth - Part I of II

10:15 AM-11:45 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS54

This symposium will bring together researchers studying mathematical models for epitaxial growth. Presentations will cover a broad range from applied analysis to experiments. Topics will include the study of formation of quantum dots and nanowire growth.

Organizer: Irene Fonseca
Carnegie Mellon University, USA

Organizer: Giovanni Leoni
Carnegie Mellon University, USA

10:15-10:40 A Continuum Model for Epitaxial Growth with Elasticity on Vicinal Surfaces

Giovanni Leoni, Carnegie Mellon University, USA; Gianni Dal Masso, SISSA, Trieste, Itlay; Irene Fonseca, Carnegie Mellon University, USA

10:45-11:10 Motion of Elastic Thin Films by Surface Diffusion with Curvature Regularization

Massimiliano Morini, Universita degli Studi di Parma, Italy

11:15-11:40 Unstable Multilayer Homoepitaxial Growth: From 2D Islands to 3D Mounds

Jim W. Evans, Iowa State University, USA

Wednesday, June 12

MS82

Mathematical and Computational Aspects of Peridynamics and Related Nonlocal Models - Part III of IV

10:15 AM-12:15 PM

Room:Symphony - 3rd Floor

For Part 2 see MS73
For Part 2 see MS91

Nonlocal models have been proposed in the past years to overcome limitations presented in local classical models. In particular, "strong" nonlocal models involving integro-differential equations, with integrands based upon differences of field quantities, provide an alternative framework to local models based upon partial differential equations. Models of this kind include peridynamics for solid mechanics and nonlocal diffusion, among others. Their novelty, however, introduces challenges from the mathematical and computational perspectives, including characterization of solutions, discretization schemes, modeling of engineering systems, description of coupled models, validation, verification, and uncertainty quantification, etc. This minisymposium invites contributions on recent developments in peridynamics and related nonlocal models.

Organizer: Pablo Seleson
University of Texas at Austin, USA

Organizer: Qiang Du
Pennsylvania State University, USA

Organizer: Michael L. Parks
Sandia National Laboratories, USA

10:15-10:40 Variable Length Scale in a Peridynamic Body

Stewart Silling, Sandia National Laboratories, USA; Pablo Seleson, University of Texas at Austin, USA

continued on next page

10:45-11:10 A Comparison of Concurrent Multiscale Methods in Peridynamics

Pablo Seleson, University of Texas at Austin, USA

11:15-11:40 Global Estimation of the Critical Time Step for Peridynamic Models

David Littlewood, Timothy Shelton, and Jesse Thomas, Sandia National Laboratories, USA

11:45-12:10 Peridigm: A New Paradigm in Computational Peridynamics

Michael L. Parks, David J. Littlewood, John A. Mitchell, and Stewart A. Silling, Sandia National Laboratories, USA

Wednesday, June 12

MS83

Theoretical Modeling and Applications of Metamaterials - Part III of IV

10:15 AM-12:15 PM

Room:Aria B - 3rd Floor

For Part 2 see MS38
For Part 2 see MS101

Dense arrays of resonant inclusions, or other substructures formed from high contrast constituents, can provide exciting bulk electromagnetic, elastodynamic, and acoustic properties that are not available in any of their constituent elements. Modeling these 'meta-' effects can become particularly challenging, especially in frequency regions in which the most interesting phenomena arise. Consequently, conventional established tools from material science need to be properly corrected and improved to rigorously capture the physics and phenomena underlying these effects. This minisymposium highlights the most recent advances in mathematical modeling, physical understanding and applications of metamaterials and their impact on the theory and applications of material science and engineering.

Organizer: Andrea Alu
University of Texas at Austin, USA

Organizer: Graeme W. Milton
University of Utah, USA

10:15-10:40 On the Computation of Optical Force and Stress in Metamaterials

C. T. Chan, Hong Kong University of Science and Technology, Hong Kong

10:45-11:10 Amplitude Activated Acoustic Metamaterial

Andrej V. Cherkaev and Elena Cherkaev, University of Utah, USA

11:15-11:40 From Asymptotic Models of Structured Plates to Control of Seismic Waves

Sebastien Guenneau, CNRS, France, and University of Liverpool, United Kingdom

11:45-12:10 Wave Propagation in Multiple Scattering Media Near Resonances: Scaling and Universality

Didier Felbacq, GES UMR CNRS, France

Wednesday, June 12

MS84

Motility and Mechanics of Biomolecular Complexes - Part III of III

10:15 AM-12:15 PM

Room:Aria A - 3rd Floor

For Part 2 see MS66

This symposium will focus on problems which draw on ideas from solid, fluid and statistical mechanics. Problems in soft materials, elastomers and biophysics are already of this nature. But, we anticipate that areas such as, complex fluids, mechanics of self-propulsion, etc., where there is significant overlap with chemistry can also benefit from mathematical approaches where Brownian motion is accounted for. Some representative topics in this symposium include: (a) Fluctuating rod models for biopolymers, (b) Mechanics of force generation in cells, (c) Swimming and self-propulsion in complex fluids, (d) Coarse-grained simulations of cellular organelles, (e) Phase transitions in macromolecular complexes.

Organizer: Prashant K. Purohit
University of Pennsylvania, USA

Organizer: Antonio DeSimone
SISSA/Trieste, Italy

10:15-10:40 Reverse Engineering the Euglenoid Movement

Marino Arroyo, Universitat Politecnica de Catalunya, Spain; Luca Heltai, SISSA, Trieste, Italy; Daniel Millan, Universitat Politècnica de Catalunya, Spain; Antonio DeSimone, SISSA/ Trieste, Italy

10:45-11:10 Ants Flow and Solidify to Build Living Rafts and Bivouacs

David Hu, Nathan Mlot, and Craig Tovey, Georgia Institute of Technology, USA

11:15-11:40 Undulatory Swimming in Complex and Heterogeneous Media

Paulo E. Arratia, University of Pennsylvania, USA

11:45-12:10 Phase Separation and Jamming of Active Particles

M. Cristina Marchetti, Syracuse University, USA

Wednesday, June 12

MS85

Multiscale Study of Defects in Solids - Part II of III

10:15 AM-12:15 PM

Room:Concerto A - 3rd Floor

For Part 1 see MS76
For Part 3 see MS94

The structures of lattice defects in solids are often responsible for many observed macroscale material properties. A full understanding of the role of defect structures typically requires a multiscale approach. This minisymposium will focus on the mathematical analysis of defect properties, accurate and robust computer simulation methods, coupled atomistic and continuum models, and coarse-graining approaches from atomistic to mesoscpoic and continuum description.

Organizer: Xiantao Li
Pennsylvania State University, USA

Organizer: Yang Xiang
Hong Kong University of Science and Technology, Hong Kong

Organizer: Zhijian Yang
Wuhan University, China

10:15-10:40 The Failure of the Continuum Theory to Evaluate the Elastic Energy of a Strained Alloy
Peter Smereka, University of Michigan, USA; Arvind Baskaran, University of California, Irvine, USA; Christian Ratsch, University of California, Los Angeles, USA

10:45-11:10 Atomistic and Continuum Simulation of Size Effects in Polycrystalline Metal Deformation
David J. Srolovitz, University of Pennsylvania, USA; Zhaoxuan Wu, Siu Sin Jerry Quek, and YongWei Zhang, Institute of High Performance Computing, Singapore

continued in next column

11:15-11:40 A Continuum Model for Dynamics of Dislocation Arrays and Applications to Low Angle Grain Boundaries
Xiaohong Zhu, Jinan University, China; Yang Xiang, Hong Kong University of Science and Technology, Hong Kong

11:45-12:10 Theory-Based Benchmarking of Blended Quasicontinuum Methods
Mitchell Luskin, University of Minnesota, USA; Xingjie Helen Li, Brown University, USA; Christoph Ortner, University of Warwick, United Kingdom; Alexander Shapeev, University of Minnesota, USA; Brian Van Koten, University of California, Los Angeles, USA

Wednesday, June 12

MS86

Stochastic Methods in Molecular Simulation: Theory and Applications - Part II of II CANCELLED

10:15 AM-12:15 PM

Wednesday, June 12

MS87

Dynamic Scaling in Models of Coarsening and Coagulation - Part II of II

10:15 AM-12:15 PM

Room:Rhapsody - 4th Floor

For Part 1 see MS60

Coarsening phenomena and cluster formation appear in many areas of materials science such as grain growth in polycrystalline materials, phase separation in alloys or dewetting of thin polymer films. Experiments often suggest that typical length scales in such systems follow universal scaling laws. A variety of mathematical models have been proposed over the last century to describe these systems, ranging from discrete and continuous mean-field type models to Cahn-Hilliard equations. A rigorous mathematical justification of scaling laws is however largely lacking and remains a major challenge. The speakers in this minisymposium will discuss new heuristic, analytical and numerical techniques to derive dynamic scaling laws in a variety of models.

Organizer: Barbara Niethammer
University of Bonn, Germany

Organizer: Joseph Conlon
University of Michigan, USA

10:15-10:40 Coarsening in Grain-boundary Networks and in a Gradient Flow of Voronoi Diagrams
Matthew Elsey, Max Planck Institut Leipzig, Germany; *Dejan Slepcev*, Carnegie Mellon University, USA

10:45-11:10 Simulations of Polycrystalline Grain Growth with Unequal Surface Energies
Matt Elsey, Courant Institute of Mathematical Sciences, New York University, USA; Selim Esedoglu, University of California, Los Angeles, USA; Peter Smereka, University of Michigan, USA

continued in next column

11:15-11:40 On the Coarsening Rates for Attachment-limited Kinetics
Christian Seis, University of Toronto, Canada

11:45-12:10 Collision Rates for the Dynamics of Interacting Slipping Droplets
Georgy Kitavtsev, Max Planck Institute for Mathematics in the Sciences, Germany

Wednesday, June 12

MS88

The Ginzburg-Landau Model and Related Topics - Part IV of V

10:15 AM-11:45 PM

Room:Minuet - 4th Floor

For Part 3 see MS61
For Part 3 see MS97

The focus of the minisymposium is on mathematical problems related to Ginzburg-Landau model with application in physics and materials science including but not limited to: superconductivity, superfluidity, liquid crystals, and polymers. The speakers in this minisymposium will describe their recent research including the development and structure of singular solutions of the Ginzburg-Landau-type problems and the dynamics of vortex motion.

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Yaniv Almog
Louisiana State University, USA

Organizer: Leonid Berlyand
Pennsylvania State University, USA

10:15-10:40 Layer Undulations in 2D and 3D Smectic Liquid Crystals
Sookyung Joo, Old Dominion University, USA

10:45-11:10 Analysis of Ferroelectric Liquid Crystals
Jinhae Park, Chungnam National University, South Korea

11:15-11:40 Phase Separation of Multiple Ginzburg-Landau Vortices Pinned by Small Holes
Leonid Berlyand, Pennsylvania State University, USA; Volodimir Rybalko, Institute for Low Temperature Physics and Engineering, Ukraine

Wednesday, June 12

MS89

Electronic Structure - Part IV of IV

10:15 AM-11:45 PM

Room:Maestro A - 4th Floor

For Part 3 see MS62

Predicting the elctronic structure of complex molecular and condensed-matter systems has been a focus of attention in chemistry and physics for decades. More recently, espceically since the advent of density functional theory (DFT), it has also become an important ingredient in materials science. Electronic structure models allows the on-the-fly computation of non-empirical and chemically specific interatomic interactions within larger-scale simulations.

Organizer: Gero Friesecke
Technische Universität München, Germany

Organizer: Eric Cances
Ecole des Ponts and INRIA, France

Organizer: Lin Lin
Lawrence Berkeley National Laboratory, USA

Organizer: Chao Yang
Lawrence Berkeley National Laboratory, USA

10:15-10:40 Adaptive Regularized Self-Consistent Field Iteration with Exact Hessian for Electronic Structure Calculation
Michael Ulbrich, Technical University of Munich, Germany; Zaiwen Wen, Shanghai Jiao Tong University, China; Andre Milzarek, Technische Universität Müchen, Germany; Hongchao Zhang, Louisiana State University, USA

10:45-11:10 Highly Accurate Numerical Solutions of Dirac Equations
Sihong Shao, Peking University, China

11:15-11:40 Coarse-Graining Density Functional Theory
Phanish Suryanarayana, California Institute of Technology, USA

Wednesday, June 12

MS90

Mathematical Crystallography: Structure-Building Principles - Part III of III

10:15 AM-12:15 PM

Room:Maestro B - 4th Floor

For Part 2 see MS36

Many crystals, such as zeolites and MOFs, consist of individual atoms or molecular building blocks with covalent bonds. Such crystals can be modeled by combinatorial and geometric structures such as geometric graphs and polyhedra, both of which are also employed for representing finite (nano-) structures, as well as rods and layers. These representations can be used for analysis of known structures, but they are increasingly used for the design of novel structures with physical and chemical properties of technological interest.

Organizer: Gregory McColm
University of South Florida, USA

Organizer: Massimo Nespolo
Université de Lorraine, France

10:15-10:40 Imprimitivity in Non-Crystallographic Nets
Jean-Guillaume Eon, Universidade Federal do Rio De Janeiro, Brazil; Montauban Moreira de Oliveira Jr, Universidade Federal Rural do Rio de Janeiro, Brazil

10:45-11:10 Tangled Nets
Stephen Hyde and Toen Castle, Australian National University, Australia; Myfanwy Evans, Universität Erlangen-Nürnberg, Germany

11:15-11:40 Self Assembly and the Structure of Matter
Richard James and Henrik van Lengerich, University of Minnesota, USA

11:45-12:10 Why Topology Matters to Crystal Engineers
Mike Zaworotko, University of South Florida, USA

Lunch Break

12:15 PM-1:30 PM

Attendees on their own

Wednesday, June 12

IP12

How Do Crystals Melt?

1:30 PM-2:15 PM

Room:Symphony - 3rd Floor

Chair: Qi Wang, University of South Carolina, USA

I will discuss the mechanism by which crystals melt. I will address the classical controversy between Born's and Lindemann's criteria for melting.

Weinan E
Princeton University, USA

Intermission

2:15 PM-2:30 PM

Wednesday, June 12

MS54

Mathematical Methods for Epitaxial Growth - Part II of II

2:30 PM-4:30 PM

Room:Rhapsody - 4th Floor

For Part 1 see MS27

This symposium will bring together researchers studying mathematical models for epitaxial growth. Presentations will cover a broad range from applied analysis to experiments. Topics will include the study of formation of quantum dots and nanowire growth.

Organizer: Irene Fonseca
Carnegie Mellon University, USA

Organizer: Giovanni Leoni
Carnegie Mellon University, USA

2:30-2:55 Equilibrium vs. Kinetic Steady States in Epitaxial Growth
Paul Patrone, University of Maryland, College Park and National Institute of Standards and Technology (NIST), USA; Dionisios Margetis, University of Maryland, College Park, USA; Russel Caflisch, University of California, Los Angeles, USA

3:00-3:25 Analytical Study of Morphology of Strained Films: Role of Misfit and Volume
Barbara Zwicknagl, University of Bonn, Germany

3:30-3:55 Lattice and Off-lattice KMC Models for Strained Epitaxial Growth
Peter Smereka and Henry A. Boateng, University of Michigan, USA; Tim Schulze, University of Tennessee, USA

4:00-4:25 Phase Field Modeling of Epitaxial Graphene Growth
Vivek Shenoy, University of Pennsylvania, USA

Wednesday, June 12

MS91

Mathematical and Computational Aspects of Peridynamics and Related Nonlocal Models - Part IV of IV CANCELLED

Wednesday, June 12

MS92

The Origins of Hysteresis in Materials - Part II of II

2:30 PM-4:00 PM

Room:Aria B - 3rd Floor

For Part 1 see MS56

Traditionally, hysteresis has been one of the most difficult structure-sensitive properties to predict. In apparently similar materials, processed similarly, the size of the hysteresis loops generated by cycling through a transformation can vary by an order-of-magnitude. Recently, ideas have been put forward by the applied mathematics community that promise to reveal a new understanding of the origins of hysteresis. These ideas have links to fundamental concepts in the calculus of variations of local minimizers, to the analysis of microstructure, and to the mathematical modeling of interfacial energy. The purpose of the minisymposium is to review and compare these timely developments.

Organizer: Richard James
University of Minnesota, USA

Organizer: David Kinderlehrer
Carnegie Mellon University, USA

2:30-2:55 Emergence of Rate Independence in Gradient Flows with Wiggly Energies
Alexander Mielke, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany; Leo Truskinovsky, École Polytechnique, France

3:00-3:25 Geometric Compatibility, Quasiconvexity and Nucleation
Konstantinos Koumatos and John Ball, University of Oxford, United Kingdom

3:30-3:55 Hysteresis in a Constrained Model for Magnetic Shape Memory Alloys
Antonio Capella Kort, Universidad Nacional Autónoma de México, Mexico

Wednesday, June 12

MS93

Active Fluids and Living Liquid Crystals - Part II of II

2:30 PM-4:30 PM

Room:Aria A - 3rd Floor

For Part 1 see MS75

Active fluids are an exciting class of complex fluids in which particles individually consume energy and collectively generate coherent translational or rotational motion. In many of these systems the individual particles can form orientational order, hence the name of living liquid crystals. The novel type of non-equilibrium dynamics makes theoretical modeling and experimental exploration of such systems extremely challenging. The goal of this symposium is to bring together a group of theorists and experimentalists from different disciplines to share the most recent results in this field, and enhance collaborations to tackle open questions in the study of such complex fluids.

Organizer: Zhenlu Cui
Fayetteville State University, USA

Organizer: M Cristina Marchetti
Syracuse University, USA

Organizer: Peter Palffy-Muhoray
Kent State University, USA

2:30-2:55 Out-of-Equilibriumness of Light Activated Colloids
Jeremy Palacci, New York University, USA; Stefano Sacanna, David Pine, and Paul Chaikin, Courant Institute of Mathematical Sciences, New York University, USA

3:00-3:25 Hydrodynamic Suppression of Phase Separation in Active Suspensions
Suzanne Fielding, Durham University, United Kingdom

3:30-3:55 Dynamics of Polyelectrolyte Gels
Lingxing Yao, University of Minnesota, USA

4:00-4:25 Analysis and Simulation of Model for Active Nematic Suspensions
Qi Wang, University of South Carolina, USA; Xiaogang Yang, Nankai University, China; Xiaofeng Yang, University of South Carolina, USA

Wednesday, June 12

MS94

Multiscale Study of Defects in Solids -- Part III of III

2:30 PM-4:00 PM

Room:Concerto A - 3rd Floor

For Part 2 see MS85

The structures of lattice defects in solids are often responsible for many observed macroscale material properties. A full understanding of the role of defect structures typically requires a multiscale approach. This minisymposium will focus on the mathematical analysis of defect properties, accurate and robust computer simulation methods, coupled atomistic and continuum models, and coarse-graining approaches from atomistic to mesoscpoic and continuum description.

Organizer: Xiantao Li
Pennsylvania State University, USA

Organizer: Yang Xiang
Hong Kong University of Science and Technology, Hong Kong

Organizer: Zhijian Yang
Wuhan University, China

2:30-2:55 The Climbing String Method for Saddle Point Search
Weiqing Ren, National University of Singapore and IHPC, Singapore

3:00-3:25 Quasiatomistic Method for Molecular Mechanics Model
Jingrun Chen and Carlos Garcia-Cervera, University of California, Santa Barbara, USA; Xiantao Li, Pennsylvania State University, USA

3:30-3:55 Crack Initiation and Propagation: A Bifurcation Study
Xiantao Li, Pennsylvania State University, USA

Wednesday, June 12

MS95

Multiscale Simulation of Materials - Part I of II

2:30 PM-4:30 PM

Room:Concerto B - 3rd Floor

For Part 2 see MS108

Multi-scale simulations are becoming an indispensable tool for modeling solids at the atomistic scale. Of particular interest are computational methodologies for bridging the scales between electronic structure, molecular mechanics and continuum mechanics. Over the past few years a theoretical foundation has begun to emerge for assessing the accuracy, efficiency and reliability of these kinds of schemes. This minisymposium will bring together experts from computational materials science, applied mathematics, and numerical analysis to review recent progress and identify new challenges for the further development of the theoretical and algorithmic basis of computational hybrid models.

Organizer: Jianfeng Lu
New York University, USA

Organizer: Mitchell Luskin
University of Minnesota, USA

Organizer: Christoph Ortner
University of Warwick, United Kingdom

2:30-2:55 The Supercell Method in Atomic Scale Simulation of Materials
Eric Cances, Ecole des Ponts and INRIA, France

3:00-3:25 Modeling Plastic Flow at Interfaces and in Glassy Polymers
Mark Robbins, Johns Hopkins University, USA

3:30-3:55 Non-Associated Plastic Flow in Crystalline Solids
John Bassani, University of Pennsylvania, USA

4:00-4:25 A New Framework for the Interpretation of Modulated Martensites in Shape Memory Alloys
Ryan S. Elliott, University of Minnesota, USA

Wednesday, June 12

MS96

Surface Evolution by Geometric Laws Controlling Interfacial Motions

2:30 PM-4:30 PM

Room:Symphony - 3rd Floor

In various fields, analyzing the mechanism of the motion of interfaces is required. The models controlling the motion of interfaces are often given by geometric evolution equations. For example, a motion of grain boundaries and a crystal growth can be described by the mean curvature flow or its flow with driving force term. Also, thermal grooving in material science and a microstructure transformation of silicon can be analyzed by the surface diffusion equation. This minisymposium will feature the mathematical and numerical analysis of the interfacial motion based on geometric evolution equations such as mentioned above.

Organizer: Yoshihito Kohsaka
Muroran Institute of Technology, Japan

2:30-2:55 On An Interfacial Motion by Surface Diffusion
Yoshihito Kohsaka, Muroran Institute of Technology, Japan

3:00-3:25 Threshold Dynamics for Networks with Arbitrary Surface Tensions
Selim Esedoglu, University of California, Los Angeles, USA; Felix Otto, Max Planck Institute for Mathematics in the Sciences, Germany

3:30-3:55 Stability of a Bunch of Spirals Evolving with An Eikonal-Curvature Flow Equation
Takeshi Ohtsuka, Gunma University, Japan

4:00-4:25 Stability and Bifurcation of Equilibria to Geometric Evolution Laws in the Axisymmetric Setting
Jeremy LeCrone, Vanderbilt University, USA

Wednesday, June 12

MS97

The Ginzburg-Landau Model and Related Topics - Part V of V

2:30 PM-4:00 PM

Room:Minuet - 4th Floor

For Part 2 see MS88
The focus of the minisymposium is on mathematical problems related to Ginzburg-Landau model with application in physics and materials science including but not limited to: superconductivity, superfluidity, liquid crystals, and polymers. The speakers in this minisymposium will describe their recent research including the development and structure of singular solutions of the Ginzburg-Landau-type problems and the dynamics of vortex motion.

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Yaniv Almog
Louisiana State University, USA

Organizer: Leonid Berlyand
Pennsylvania State University, USA

2:30-2:55 Hydrodynamic limit of Gross-Pitaevksy vortices on the plane
Daniel Spirn, University of Minnesota, USA

3:00-3:25 The Hydrodynamic Limit of the Parabolic Ginzburg-Landau Equation
Matthias Kurzke, University of Bonn, Germany; Daniel Spirn, University of Minnesota, USA

3:30-3:55 Asymptotic Analysis of Minimizers for the Lawrence-Doniach Energy
Patricia Bauman and Guanying Peng, Purdue University, USA

Wednesday, June 12

MS98

Advances in Modeling and Computation of Thin Liquid Films in Materials Science - Part II of II

2:30 PM-4:30 PM

Room:Maestro A - 4th Floor

For Part 1 see MS80
We propose a two-session minisymposium focusing on modeling and numerical simulation of thin films. This minisymposium will bring together mathematicians, physicists, and engineers at the frontier of the research in thin liquid films in materials science. The two-session minisymposium will allow vibrant and timely discussion and rich exchange of ideas. Topics will include: new computational and analytical methods for modeling interfaces and contact lines, coupling between atomic level and continuum simulations, self and directed assembly, liquid-crystal statics and dynamics, and applications to micro- and nano-fluidics. Speakers will include distinguished international experts including experimental researchers, as well as junior and early-career researchers with expertise in thin films.

Organizer: Shahriar Afkhami
New Jersey Institute of Technology, USA

Organizer: Linda Cummings
New Jersey Institute of Technology, USA

Organizer: Lou Kondic
New Jersey Institute of Technology, USA

2:30-2:55 Modeling and Simulation of Nematic Liquid Crystal Films
Linda Cummings, New Jersey Institute of Technology, USA

3:00-3:25 Directed, Liquid Phase Assembly of Patterned Metallic Films by Pulsed Laser Dewetting
Philip D. Rack, University of Tennessee, USA

3:30-3:55 Stability of Liquid Rings
Lou Kondic, New Jersey Institute of Technology, USA

4:00-4:25 Fingering Instability Down the Outside of a Vertical Cylinder
Linda Smolka, Bucknell University, USA

Wednesday, June 12

MS99

Morphological Evolution of Crystalline Surfaces, Thin Films, and Clusters - Part II of II

2:30 PM-4:30 PM

Room:Maestro B - 4th Floor

For Part 1 see MS72

Non-equilibrium morphological evolution of crystalline surfaces and thin films, and of supported or liquid-phase clusters, is a key element of nanotechnology. Despite some progress, many related phenomena remain poorly understood. A central issue is to reconcile descriptions across several time and length scales, from atomistic to mesoscale to continuum. Unresolved problems include far-from-equilibrium growth shapes during self-assembly of clusters by surface deposition or in liquid-phase synthesis, multilayer growth and faceting, stochastic fluctuations of surface features, and post-growth relaxation and stability of nanostructures. This minisymposium reviews recent advances in modeling, analysis and simulation.

Organizer: Jim W. Evans
Iowa State University, USA

Organizer: Dionisios Margetis
University of Maryland, College Park, USA

2:30-2:55 Aspects of Faceting in Epitaxial Relaxation
Dionisios Margetis, University of Maryland, College Park, USA

3:00-3:25 Symmetry-Breaking in Shape Transitions of Epitaxially-Strained Islands
Brian J. Spencer, State University of New York at Buffalo, USA; Jerry Tersoff, IBM T.J. Watson Research Center, USA

continued in next column

3:30-3:55 Kinetic Monte Carlo Models for Nanoclusters and Dendrites
Tim Schulze, University of Tennessee, USA

4:00-4:25 Effect of Melt Flow on Morphological Evolution of Nanocrystal Nucleates
Arvind Baskaran, University of California, Irvine, USA; Aparna Baskaran, Brandeis University, USA; John Lowengrub, University of California, Irvine, USA

Coffee Break

4:30 PM-5:00 PM

Room:Assembly - 3rd Floor

Wednesday, June 12

MS100

Material Modelling and Gradient Flows

5:00 PM-7:00 PM

Room:Symphony - 3rd Floor

Gradient flows, in the classical setting, has been an important subject of interest due to the wide variety of applications they have such as heat conduction, reaction-diffusion systems and mean curvature flow. The variational structure one can use in gradient systems makes it possible to describe a large class of phenomena including evolution of microstructure in materials, damage and fracture. The aim of our minisymposium is to link the theory of gradient flows with different nonlinear models for materials, and review new application fields and recent progress on the subject.

Organizer: Yasemin Sengul
Ozyegin University, Turkey

5:00-5:25 An Approach to Nonlinear Viscoelasticity Via Metric Gradient Flows
Yasemin Sengul, Ozyegin University, Turkey; Alexander Mielke, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany; Christoph Ortner, University of Warwick, United Kingdom

5:30-5:55 Quasistatic Nonlinear Viscoelasticity and Gradient Flows
John Ball, University of Oxford, United Kingdom; Yasemin Sengul, Ozyegin University, Turkey

6:00-6:25 Existence Results for Generalized Gradient Systems with Applications to Finite-Strain Elasticity
Alexander Mielke, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany; *Riccarda Rossi*, University of Brescia, Italy; Giuseppe Savare', University of Pavia, Italy

6:30-6:55 Gradient Structures and Geodesic Convexity for Reaction-Diffusion System
Matthias Liero, and Alexander Mielke, Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany

Wednesday, June 12

MS101

Theoretical Modeling and Applications of Metamaterials - Part IV of IV

5:00 PM-7:00 PM

Room:Aria B - 3rd Floor

For Part 3 see MS83

Dense arrays of resonant inclusions, or other substructures formed from high contrast constituents, can provide exciting bulk electromagnetic, elastodynamic, and acoustic properties that are not available in any of their constituent elements. Modeling these 'meta-' effects can become particularly challenging, especially in frequency regions in which the most interesting phenomena arise. Consequently, conventional established tools from material science need to be properly corrected and improved to rigorously capture the physics and phenomena underlying these effects. This minisymposium highlights the most recent advances in mathematical modeling, physical understanding and applications of metamaterials and their impact on the theory and applications of material science and engineering.

Organizer: Andrea Alu
University of Texas at Austin, USA

Organizer: Graeme W. Milton
University of Utah, USA

5:00-5:25 Bloch Waves Expansion for High Contrast Homogenization
Guy Bouchitte, Universite de Toulon et du Var, France

5:30-5:55 Plasmonic Waves Allow Perfect Transmission of Light Through Sub-Wavelength Holes
Ben Schweizer, TU Dortmund, Germany

6:00-6:25 Controlling the Phase and Power Flow of Electromagnetic Fields with Metamaterials
Anthony Grbic and Gurkan Gok, University of Michigan, Ann Arbor, USA

6:30-6:55 Cloud Computing for Nanophotonics: Multiphysics and Ultra-Fast Solvers
Alexander V. Kildishev, Purdue University, USA

Wednesday, June 12

MS102

Geometrical Instabilities in Soft Materials - Part II of II

5:00 PM-7:00 PM

Room:Aria A - 3rd Floor

For Part 1 see MS65

The macroscopic properties and failure mechanisms of a truly diverse variety of solids are known to be the eventual manifestation of instabilities that occur across a broad range of length scales. This symposium will address recent advances in the mathematical modeling of such local instabilities. Topics of particular interest include: i) Cavitation and fracture; ii) Creasing and wrinkling; iii) Microstructural instabilities in heterogeneous material systems responsive to coupled stimuli such as electrostrictive and liquid crystal elastomers.

Organizer: Oscar Lopez-Pamies
University of Illinois at Urbana-Champaign, USA

Organizer: Scott Spector
Southern Illinois University, USA

5:00-5:25 Cavitation in Rubber: An Elastic Instability of a Fracture Phenomenon?
Oscar Lopez-Pamies and Victor Lefevre, University of Illinois at Urbana-Champaign, USA

5:30-5:55 Quasistatic Evolution of Cavities in Nonlinear Elasticity
Carlos Mora-Corral, Universidad Autonoma de Madrid, Spain

6:00-6:25 A Regularized Penalty-multiplier Method for the Computation of Fracture Surfaces in Strain Space
J. Sivaloganathan, University of Bath, United Kingdom; *Pablo Negron*, University of Puerto Rico, Humacao, Puerto Rico

6:30-6:55 On the Global Stability of Elastic Cylinders under Tension
J. Sivaloganathan, University of Bath, United Kingdom; Scott Spector, Southern Illinois University, USA

Wednesday, June 12

MS103

Mathematical Modeling of Dislocations in Crystalline Solids - Part II of II

5:00 PM-7:00 PM

Room:Concerto A - 3rd Floor

For Part 1 see MS67

The focus of the minisymposium will be on mathematical issues in studies of dislocations - defects in a crystalline lattice structure that play an important role in defining macroscopic properties of solids. The speakers will discuss their recent results in modeling of dislocations at all levels - from microscopic to macroscopic - and on exploring connections between various length- and timescales.

Organizer: Dmitry Golovaty
University of Akron, USA

Organizer: Malena I. Espanol
University of Akron, USA

5:00-5:25 Multiscale Problems in Dislocation Theory
Lucia Scardia, University of Glasgow, Scotland, UK; Mark Peletier, Ron Peerlings, and Marc Geers, Technische Universiteit Eindhoven, The Netherlands; Caterina Zeppieri, Universität Münster, Germany

5:30-5:55 Peierls Stress in Continuum Dislocation Mechanics
Xiaohan Zhang and *Amit Acharya*, Carnegie Mellon University, USA

6:00-6:25 Continuum Dislocation Theory for Modeling Size Effects in Crystal Plasticity
Dennis M. Kochmann, California Institute of Technology, USA; Chau Le, Ruhr-Universität Bochum, Germany

6:30-6:55 Asymptotic Analysis and Dynamics of a System of Straight Dislocations
Adriana Garroni, Universita di Roma "La Sapienza," Italy; Roberto Alicandro, Università di Cassino, Italy; Lucia De Luca, Sapienza – Università di Roma, Italy; Marcello Ponsiglione, Università di Roma I, Italy

Wednesday, June 12

MS104

Analysis and Computations for Non-equilibrium Molecular Systems - Part II of II

5:00 PM-7:00 PM

Room:Concerto B - 3rd Floor

For Part 1 see MS23

The minisymposium will address recent and ongoing developments in analysis and simulation of non-equilibrium molecular systems for materials design. In particular, we will discuss the fidelity and sensitivity of atomistic and coarse-grained stochastic models in transient and stationary regimes. Mathematical topics will include information-theoretic tools, as well as non-equilibrium statistical mechanics techniques and computational methods for analysing driven extended stochastic systems.

Organizer: Markos A. Katsoulakis
University of Massachusetts, Amherst, USA

Organizer: Petr Plechac
University of Delaware, USA

5:00-5:25 Measuring Irreversibility in Numerical Schemes for Langevin Equations
Luc Rey-Bellet, University of Massachusetts, USA

5:30-5:55 Pathwise Sensitivity Analysis of Complex Stochastic Dynamics Based on Relative Entropy Rate
Yiannis Pantazis, University of Massachusetts, Amherst, USA

6:00-6:25 A Two Scale Proof of the Eyring-Kramers Formula
Georg Menz, Stanford University, USA

6:30-6:55 Multiscale KMC-DFT Simulation on Bimetallic Catalysts
Wei Guo, University of Delaware, USA

Wednesday, June 12

MS105

Phase Field Methods in Materials Science: Recent Developments - Part II of II

5:00 PM-7:00 PM

Room:Rhapsody - 4th Floor

For Part 1 see MS51

Phase field methods have evolved into a useful practical tool as a wide assortment of materials science problems have been addressed using this methodology. As computational power increases, the potential of this methodology is enhanced. Correspondingly, there is also a greater need for modeling and theoretical results. This session will focus on theoretical and computational issues in phase field equations and related methods involving a diffuse interface.

Organizer: Steven M. Wise
University of Tennessee, USA

Organizer: Gunduz Caginalp
University of Pittsburgh, USA

Organizer: Emre Esenturk
Pohang University of Science and Technology, South Korea

5:00-5:25 Two Phase Flow in Porous Media
Xiaoming Wang, Florida State University, USA

5:30-5:55 Gpu Parallelized Spectral Methods for Phase-Field and Phase-Field-Crystal Models
Feng Chen, Brown University, USA

6:00-6:25 A Numerical Analysis of the Cahn-Hilliard Equation in a Domain with Non Permeable Walls
Laurence Cherfils, Universitè de la Rochelle, France

6:30-6:55 Convex Splitting Methods for Nonlocal Models of Phase Separation
Zhen Guan, University of California, Irvine, USA

Wednesday, June 12

MS106

Geometric Variational Problems with Long-range Interactions - Part II of II

5:00 PM-7:00 PM

Room:Minuet - 4th Floor

For Part 1 see MS71

Variational problems involving competing short-range and long-range interactions often arise in the studies of phase transitions in different materials and, more broadly, in systems exhibiting energy driven pattern formation. In the recent few years, there has been much work on two basic paradigms: The Ohta-Kawasaki energy functional, which arises as a model of self-assembly in diblock copolymer melts, and isoperimetric problems in the presence of long-range forces. This minisymposium will focus on recent analytical advances in these and related problems, with a focus on geometric properties on energy minimizing interfaces. Extensions to diffuse interface models and related problems will also be explored.

Organizer: Rustum Choksi
McGill University, Canada

Organizer: Cyrill B. Muratov
New Jersey Institute of Technology, USA

5:00-5:25 On the Shape of Charged Drops: an Isoperimetric Problem with a Competing Non-local Term.
Hans Knuepfer, University of Bonn, Germany

5:30-5:55 Minimality via Second Variation for a Nonlocal Isoperimetric Problem
Massimiliano Morini, Universita degli Studi di Parma, Italy

6:00-6:25 A Double Bubble Solution in a Ternary System with Inhibitory Long Range Interaction
Xiaofeng Ren, George Washington University, USA

6:30-6:55 Energy Driven Pattern Formation in a Non-local Ginzburg-Landau/Cahn-Hilliard Energy
Dorian Goldman, Courant Institute of Mathematical Sciences, New York University, USA

Wednesday, June 12

MS107

From Microscopic to Continuum: Variational Multiscale Methods: Part IV of IV

5:00 PM-7:00 PM

Room:Maestro A - 4th Floor

For Part 3 see MS81

This minisymposium addresses new results in the application of variational multiscale methods to systems related to materials science. Different approaches to coupling of the two extreme scales: the microscopic and the continuum will be at the center of the attention. Other recent advances with mesoscopic and multiscale character, such as: homogenization of composite materials, emergence of wrinkling patterns driven by loading or growth, prediction of dislocations and fracture, dimension reduction, microstructures and thin films of nematic liquid crystal, will be discussed. The objective of this minisymposium is to bring together experts and younger scientists from applied mathematics and mechanics to view advances and challenges from different perspectives.

Organizer: Marta Lewicka
University of Pittsburgh, USA

Organizer: Anja Schloemerkemper
University of Würzburg, Germany

5:00-5:25 Asymptotics of a Prototype Lattice Energy under an Impenetrability Constraint
Maria Stella Gelli, Universita' di Pisa, Italy; Andrea Braides, University of Rome, Italy

5:30-5:55 Homogenization of the Kirchhoff Bending Theory for Plates
Heiner Olbermann, University of Bonn, Germany

6:00-6:25 From Wrinkles to Scars: Universality of Stress Collapse in Confined Crystalline Sheets
Benjamin Davidovich and Gregory M. Grason, University of Massachusetts, Amherst, USA

6:30-6:55 Effective Behavior of Thin Films of Liquid Crystal Elastomers
Kaushik Bhattacharya, California Institute of Technology, USA

Wednesday, June 12

MS108

Multiscale Simulation of Materials - Part II of II

5:00 PM-7:00 PM

Room:Maestro B - 4th Floor

For Part 1 see MS95

Multi-scale simulations are becoming an indispensable tool for modeling solids at the atomistic scale. Of particular interest are computational methodologies for bridging the scales between electronic structure, molecular mechanics and continuum mechanics. Over the past few years a theoretical foundation has begun to emerge for assessing the accuracy, efficiency and reliability of these kinds of schemes. This minisymposium will bring together experts from computational materials science, applied mathematics, and numerical analysis to review recent progress and identify new challenges for the further development of the theoretical and algorithmic basis of computational hybrid models.

Organizer: Jianfeng Lu
New York University, USA

Organizer: Mitchell Luskin
University of Minnesota, USA

Organizer: Christoph Ortner
University of Warwick, United Kingdom

5:00-5:25 Energy-Based Atomistic-to-Continuum Coupling
Alexander V. Shapeev, University of Minnesota, USA

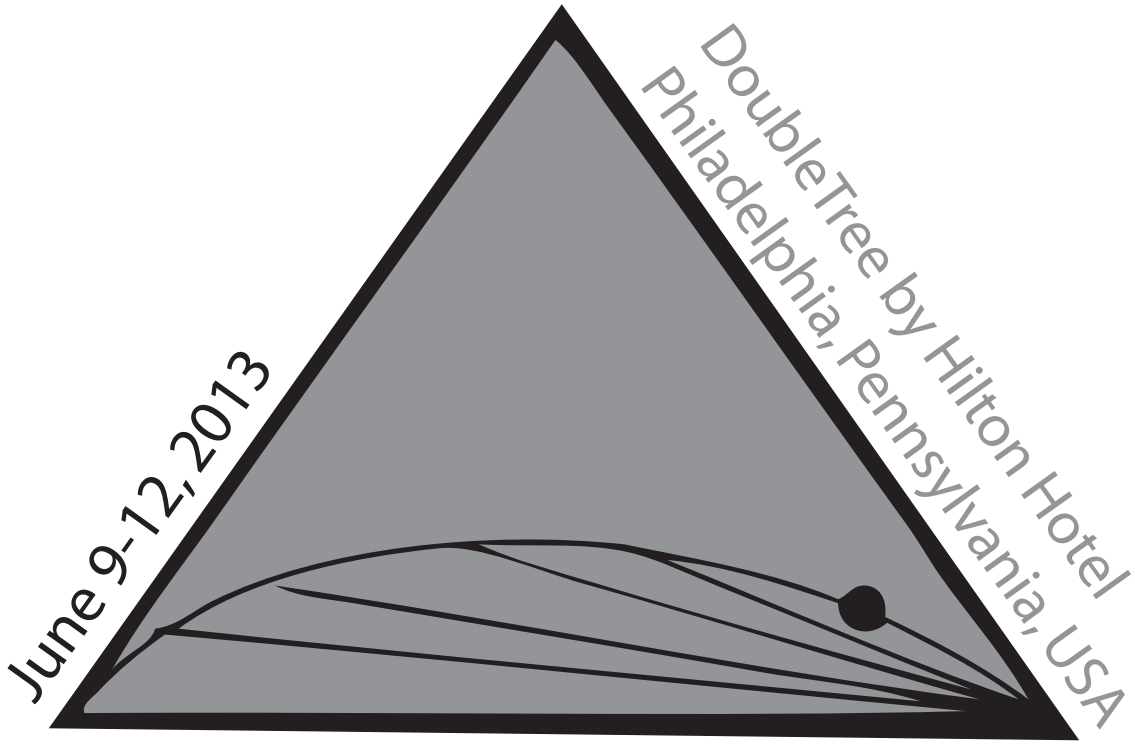
5:30-5:55 Consistent Atomistic/ Continuum Coupling Methods
Lei Zhang, Shanghai Jiao Tong University, China; Christoph Ortner, University of Warwick, United Kingdom

6:00-6:25 Numerical Analysis of the Blended Quasicontinuum Method
Brian Van Koten, University of California, Los Angeles, USA

6:30-6:55 An Optimization Based Atomistic-to-Continuum Coupling Method
Derek Olson, University of Minnesota, USA; Pavel Bochev, Sandia National Laboratories, USA; Mitchell Luskin and Alexander V. Shapeev, University of Minnesota, USA

Notes

MS13 Abstracts



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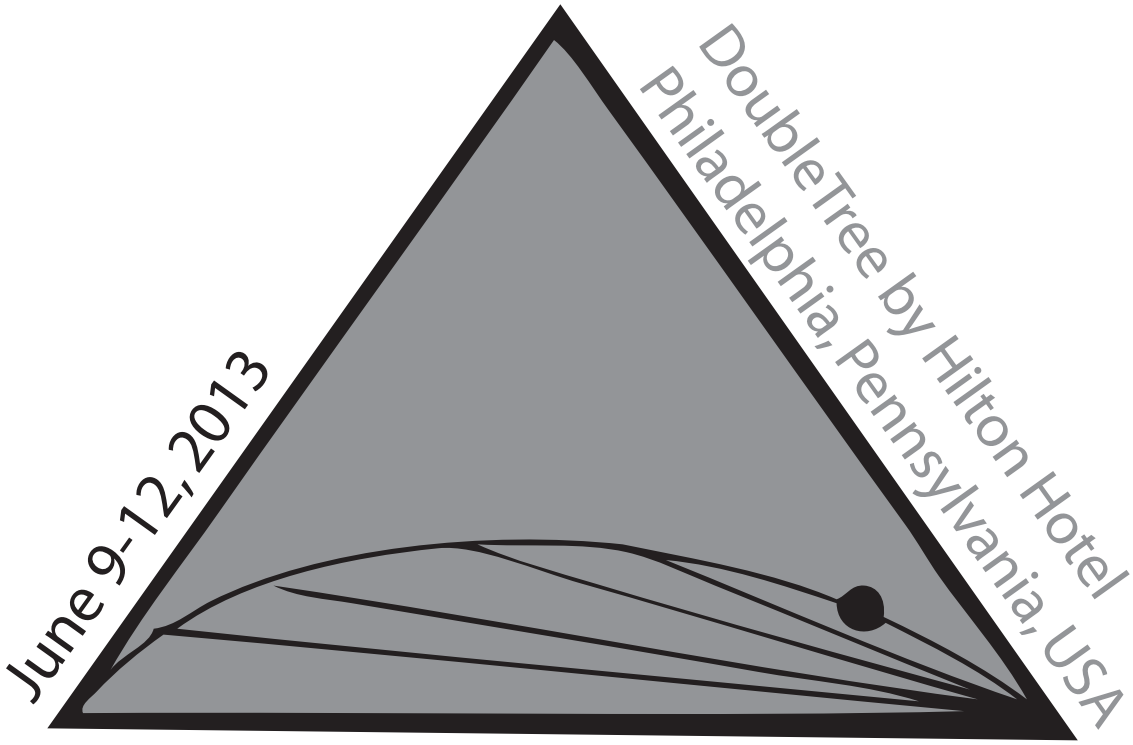
Abstracts are printed as submitted by the authors.

last page of abstracts

Organizer and Speaker Index



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MS13 Budget

Conference Budget
SIAM Conference on Mathematical Aspects of Materials Science
June 9-12, 2013
Philadelphia, PA

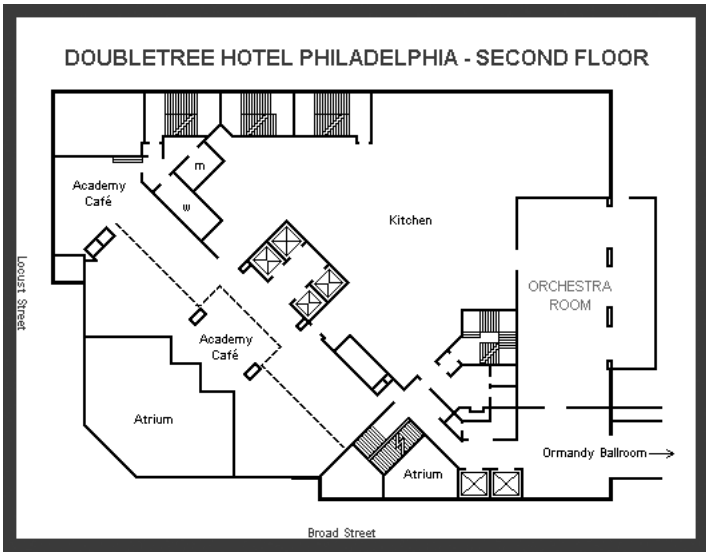
Expected Paid Attendance 330

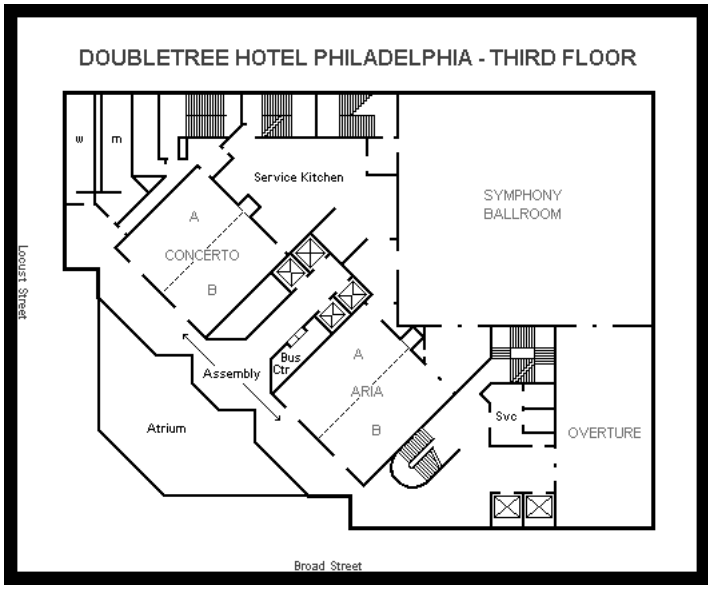
Revenue		
Registration Income		$106,670
Total		$106,670
Expenses		
Printing		$2,900
Organizing Committee		$2,200
Invited Speakers		$14,600
Food and Beverage		$17,600
AV Equipment and Telecommunication		$13,700
Advertising		$7,400
Conference Labor (including benefits)		$24,914
Other (supplies, staff travel, freight, misc.)		$1,200
Administrative		$9,408
Accounting/Distribution & Shipping		$6,602
Information Systems		$8,992
Customer Service		$3,386
Marketing		$5,504
Office Space (Building)		$3,693
Other SIAM Services		$4,119
	Total	$126,218
Net Conference Expense		($19,548)
Support Provided by SIAM		$19,548
		$0

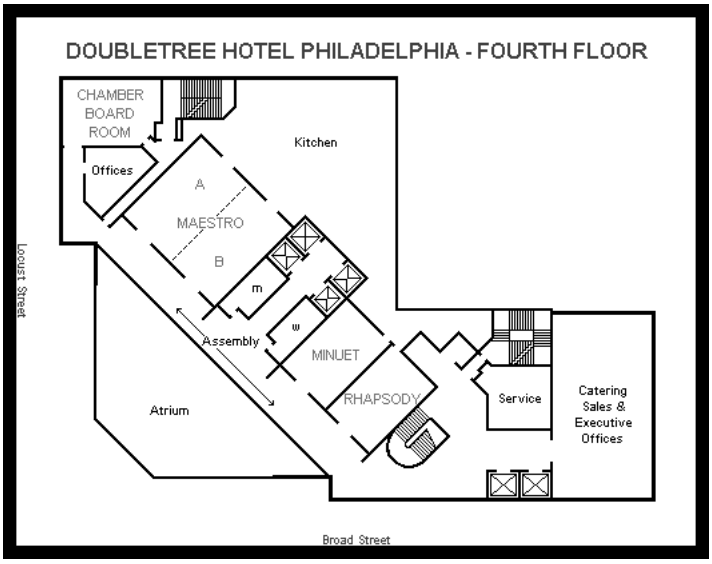
Estimated Support for Travel Awards not included above:

Post Docs and Students	12	$9,120

DoubleTree by Hilton Hotel Floor Plans







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