Final Program and Abstracts



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.

The activity group sponsors the triennial SIAM Conference on Mathematical Aspects of Materials Science and minisymposia at the SIAM annual meetings. It also maintains a wiki, a member directory, and an electronic mailing list.



MS16 Mobile App

Scan the QR code with any QR reader and download the TripBuilder EventMobileTM app to your iPhone, iPad, iTouch or Android mobile device.

You can also visit www.tripbuildermedia.com/apps/siam2016events



Society for Industrial and Applied Mathematics 3600 Market Street, 6th Floor Philadelphia, PA 19104-2688 USA Telephone: +1-215-382-9800 Fax: +1-215-386-7999 Conference Email: meetings@siam.org Conference Web: www.siam.org/meetings/ Membership and Customer Service: (800) 447-7426 (US& Canada) or +1-215-382-9800 (worldwide)

www.siam.org/meetings/ms16

2016 SIAM Conference on Mathematical Aspects of Materials Science

Table of Contents

Program-At-A-Glance
See separate handout
General Information2
Get-togethers
Invited Plenary Presentations 6
Program Schedule 11
Poster Session 44
Abstracts
Speaker and Organizer Index 191
Conference Budget
Inside Back Cover
Hotel Meeting Room Map
Outside Back Cover

Organizing Committee Co-chairs

Qiang Du Columbia University, USA

David Srolovitz University of Pennsylvania, USA

Organizing Committee

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

Dmitry Golovaty University of Akron, USA

Robert Lipton Louisiana State University, USA

Kristin Persson University of California, Berkeley and Lawrence Berkeley National Laboratory, USA

Ellad Tadmor University of Minnesota, USA

Florian Theil University of Warwick, United Kingdom

Axel Voigt Technische Universität Dresden, Germany

Peter Voorhees Northwestern University, USA

Jonathan Weare University of Chicago, USA

Yang Xiang

The Hong Kong University of Science and Technology, Hong Kong

Pingwen Zhang Peking University, China

Dana Zöllner University of Magdeburg, Germany

SIAM Registration Desk

The SIAM registration desk is located in the Society Hill Ballroom Foyer. It is open during the following hours:

> Saturday, May 7 4:00 PM - 8:00 PM

Sunday, May 8 7:00 AM - 5:30 PM

Monday, May 9 7:30 AM - 5:30 PM

Tuesday, May 10 7:30 AM - 5:30 PM

Wednesday, May 11 7:30 AM - 5:30 PM

Thursday, May 12 7:30 AM - 3:30 PM

Hotel Address

Sheraton Society Hill Hotel 1 Dock Street Philadelphia, Pennsylvania 19106

Hotel Telephone Number

To reach an attendee or leave a message, call +1-215-238-6000. If the attendee is a hotel guest, the hotel operator can connect you with the attendee's room.

Hotel Check-in and Checkout Times

Check-in time is 3:00 PM. Check-out time is 12:00 PM.

Child Care

The Philadelphia Convention and Visitors Bureau recommend The Philadelphia Nanny Network (*http:// www.nannyagency.com/*) and Your Other Hands (*http://www.yourotherhands.com/ services.html*) for attendees interested in child care services. Attendees are responsible for making their own child care arrangements.

Corporate Members and Affiliates

SIAM corporate members provide their employees with knowledge about, access to, and contacts in the applied mathematics and computational sciences community through their membership benefits. Corporate membership is more than just a bundle of tangible products and services; it is an expression of support for SIAM and its programs. SIAM is pleased to acknowledge its corporate members and sponsors. In recognition of their support, nonmember attendees who are employed by the following organizations are entitled to the SIAM member registration rate.

Corporate Institutional Members

The Aerospace Corporation Air Force Office of Scientific Research Amazon Aramco Services Company Bechtel Marine Propulsion Laboratory The Boeing Company CEA/DAM Department of National Defence (DND/ CSEC) DSTO- Defence Science and Technology Organisation Hewlett-Packard Huawei FRC French R&D Center **IBM** Corporation IDA Center for Communications Research, La Jolla **IDA** Center for Communications Research, Princeton

Institute for Defense Analyses, Center for Computing Sciences

Lawrence Berkeley National Laboratory

Lawrence Livermore National Labs

Lockheed Martin

Los Alamos National Laboratory

Max-Planck-Institute for Dynamics of Complex Technical Systems

Mentor Graphics

National Institute of Standards and Technology (NIST)

National Security Agency (DIRNSA)

Naval PostGrad

Oak Ridge National Laboratory, managed by UT-Battelle for the Department of Energy

Sandia National Laboratories

Schlumberger-Doll Research

United States Department of Energy

U.S. Army Corps of Engineers, Engineer Research and Development Center US Naval Research Labs

List current April 2016.

Funding Agencies

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



Leading the applied mathematics community

Join SIAM and save!

SIAM members save up to \$130 on full registration for the 2016 SIAM Conference on Mathematical Aspects of Materials Science! Join your peers in supporting the premier professional society for applied mathematicians and computational scientists. SIAM members receive subscriptions to *SIAM Review, SIAM News and SIAM Unwrapped,* and enjoy substantial discounts on SIAM books, journal subscriptions, and conference registrations.

If you are not a SIAM member and paid the Non-Member or Non-Member

Mini Speaker/Organizer rate to attend the conference, you can apply the difference between what you paid and what a member would have paid (\$130 for a Non-Member and \$65 for a Non-Member Mini Speaker/Organizer) towards a SIAM membership. Contact SIAM Customer Service for details or join at the conference registration desk.

If you are a SIAM member, it only costs \$10 to join the SIAM Activity Group on the Mathematical Aspects of Materials Science (SIAG/MS). As a SIAG/MS member, you are eligible for an additional \$10 discount on this conference, so if you paid the SIAM member rate to attend the conference, you might be eligible for a free SIAG/MS membership. Check at the registration desk.

Free Student Memberships are available to students who attend an institution that is an Academic Member of SIAM, are members of Student Chapters of SIAM, or are nominated by a Regular Member of SIAM.

Join onsite at the registration desk, go to *www.siam.org/joinsiam* to join online or download an application form, or contact SIAM Customer Service: Telephone: +1-215-382-9800 (worldwide); or 800-447-7426 (U.S. and Canada only)

Fax: +1-215-386-7999

E-mail: membership@siam.org

Postal mail: Society for Industrial and Applied Mathematics, 3600 Market Street, 6th floor, Philadelphia, PA 19104-2688 USATelephone: +1-215-382-9800 (worldwide); or 800-447-7426 (U.S. and Canada only)

Standard Audio/Visual Set-Up in Meeting Rooms

SIAM does not provide computers for any speaker. When giving an electronic presentation, speakers must provide their own computers. SIAM is not responsible for the safety and security of speakers' computers.

The Plenary Session Room will have two (2) screens, one (1) data projector and one (1) overhead projector. The data projectors support VGA connections only. Presenters requiring an HDMI or alternate connection must provide their own adaptor.

All other concurrent/breakout rooms will have one (1) screen and one (1) data projector. The data projectors support VGA connections only. Presenters requiring an HDMI or alternate connection must provide their own adaptor.

If you have questions regarding availability of equipment in the meeting room of your presentation, please see a SIAM staff member at the registration desk.

Internet Access

Complimentary wireless Internet access will be available for SIAM attendees in the meeting space, guestrooms in the SIAM room block, and public areas of the hotel.

In addition, a limited number of computers with Internet access will be available during registration hours.

Registration Fee Includes

- Admission to all technical sessions
- Business Meeting (open to SIAG/ MS members)
- Coffee breaks daily
- Poster Session
- Room set-ups and audio/visual equipment
- 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 Monday, May 9, from 8:00 PM – 10:00 PM. Presenters are requested to put up their posters no later than 8:00 PM on Monday, the official start time of the session. Boards and push pins will be available to presenters beginning Saturday, May 7, at 5:00 PM. For information about preparing a poster, please visit *http://www.siam.org/ meetings/guidelines/presenters.php.*

Note: Any poster presenter who fails to show and present a confirmed presentation will be considered a no-show. No-shows will be billed \$65 per accepted poster.

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 12:00 PM on Thursday.

Name Badges

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:

Cynthia Phillips, SIAM Vice President for Programs (*vpp@siam.org*).

Get-togethers

- Welcome Reception Saturday, May 7
 6:00 PM - 8:00 PM
- **Poster Session** Monday, May 9 8:00 PM - 10:00 PM

Business Meeting (open to SIAG/MS members) Tuesday, May 10 1:30 PM - 2:15 PM

Complimentary beverages will be served.

Statement on Inclusiveness

As a professional society, SIAM is committed to providing an inclusive climate that encourages the open expression and exchange of ideas, that is free from all forms of discrimination, harassment, and retaliation, and that is welcoming and comfortable to all members and to those who participate in its activities. In pursuit of that commitment, SIAM is dedicated to the philosophy of equality of opportunity and treatment for all participants regardless of gender, gender identity or expression, sexual orientation, race, color, national or ethnic origin, religion or religious belief, age, marital status, disabilities, veteran status, field of expertise, or any other reason not related to scientific merit. This philosophy extends from SIAM conferences, to its publications, and to its governing structures and bodies. We expect all members of SIAM and participants in SIAM activities to work towards this commitment.

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.

Recording of Presentations

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 #SIAMMS16.



The SIAM 2016 Events Mobile App Powered by TripBuilder®

To enhance your conference experience, we're providing a state-of-the-art mobile app to give you important conference information right at your fingertips. With this TripBuilder EventMobile[™] app, you can:

• Create your own custom schedule

• View Sessions, Speakers, Exhibitors and more

• Take notes and export them to your email

• View Award-Winning TripBuilder Recommendations for the meeting location

• Get instant Alerts about important conference info



SIAM 2016 Events Mobile App

Scan the QR code with any QR reader and download the TripBuilder EventMobileTM app to your iPhone, iPad, iTouch or Android mobile device.

To access the app or the HTML 5 version, visit *www.tripbuildermedia*. *com/apps/siam2016events*

Invited Plenary Speakers

** All Invited Plenary Presentations will take place in Society Hill Ballroom B,C,D,E**

Sunday, May 8 8:15 AM - 9:00 AM

IP1 Effective Behavior of Random Media: An Error Analysis Felix Otto, Max Planck Institute for Mathematics in the Sciences, Germany

9:00 AM - 9:45 AM

IP2 Stack `em Up: Growth, Coarsening, and Alignment of Compositional Domains in Lipid Bilayer Membrane Systems Mikko Haataja, Princeton University, USA

1:30 PM - 2:15 PM

IP3 Topology and Geometry of Dislocation Networks under Extreme Straining **Vasily Bulatov**, Lawrence Livermore National Laboratory, USA

Monday, May 9

8:15 AM - 9:00 AM

IP4 On the Trail of Hipsters and Robber Barons: Probing Microstructural Evolution Using Time-Resolved 3D X-Ray Imaging

Carl E. Krill III, Ulm University, Germany

9:00 AM - 9:45 AM

IP5 Theory and Challenges for Microstructure Evolution David Kinderlehrer, Carnegie Mellon University, USA

Invited Plenary Speakers

** All Invited Plenary Presentations will take place in Society Hill Ballroom B,C,D,E**

Tuesday, May 10 8:15 AM - 9:00 AM

IP6 Transforming Molecular Modelling with Applied Mathematics Gábor Csányi, University of Cambridge, United Kingdom

9:00 AM - 9:45 AM

IP7 Epitaxial Graphene Growth John Lowengrub, University of California, Irvine, USA

> Wednesday, May 11 8:15 AM - 9:00 AM

IP8 A Study of Speed Dependent Contact Angle Hysteresis Xiaoping Wang, Hong Kong University of Science and Technology, Hong Kong

9:00 AM - 9:45 AM

IP9 Mathematical Crystallography and Virology: Group and Graph Theoretical Approaches for the Characterization of Viruses Structure Reidun Twarock, University of York, United Kingdom

1:30 PM - 2:15 PM

IP10 Title Not Available Christof Schütte, Freie Universität Berlin, Germany

Invited Plenary Speakers

** All Invited Plenary Presentations will take place in Society Hill Ballroom B,C,D,E**

Thursday, May 12 8:15 AM - 9:00 AM

IP11 Issues in the Multiscale Modeling and Methods of Solids Pingbing Ming, Chinese Academy of Sciences, China

9:00 AM - 9:45 AM

IP12 The 3D Structural Geometry of Nanoporous Gold and its Influence on Mechanical ResponseErica Lilleodden, Helmholtz Zentrum Geesthacht, Germany

1:30 PM - 2:15 PM

IP13 Can You Print Your Toughness? Kaushik Bhattacharya, California Institute of Technology, USA



SIAM Presents is an audio-visual archive

comprised of more than 2,000 presentations posted in over 40 searchable topics, including:

- algebraic geometry
- atmospheric and oceanographic science
- computational science
- data mining
- geophysical science
- optimization
- uncertainty quantification and more...

The collection, Featured Lectures from our Archives, includes audio and slides from more than 30 conferences since 2008, including talks by invited and prize speakers, select minisymposia, and minitutorials. Presentations from SIAM meetings are being added throughout the year.

In addition you can view short video clips of speaker interviews from sessions at Annual Meetings starting in 2010.

Plans for adding more content are on the horizon. Keep an eye out!

The audio, slide, and video presentations are part of SIAM's outreach activities to increase the public's awareness of mathematics and computational science in the real world, and to bring attention to exciting and valuable work being done in the field. Funding from SIAM, the National Science Foundation, and the Department of Energy was used to partially support this project.



New presentations are posted every few months as the program expands with sessions from additional SIAM meetings. Users can search for presentations by category, speaker name, and/or key words.

www.siam.org/meetings/presents.php

Society for Industrial and Applied Mathematics • 3600 Market Street, 6th Floor • Philadelphia, PA 19104-2688 USA Phone: +1-215-382-9800 • Fax +1-215-386-7999 • service@siam.org • www.siam.org

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

http://www.siam.org/activity/materials_science/index.php

A GREAT WAY TO GET INVOLVED!



ACTIVITIES INCLUDE:

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

BENEFITS OF SIAG/MS MEMBERSHIP:

- Listing in the SIAG's online-only 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!

SIAG/MS OFFICERS 2015-2016

- Chair: Qiang Du, Columbia University
- · Vice Chair: John Lowengrub, University of California, Irvine
- Secretary: Maria Emelianenko, George Mason University

TO JOIN:

SIAG/MS: my.siam.org/forms/join_siag.htm SIAM: www.siam.org/joinsiam

Collaborate and interact with mathematicians and applied scientists whose work involves Mathematical Aspects of materials science.



MS16 Program



SIAM Conference on Mathematical Aspects of Materials Science

Saturday, May 7

Registration 4:00 PM-8:00 PM Room:Society Hill Ballroom Foyer

Welcome Reception

6:00 PM-8:00 PM Room:Hamilton Room



Sunday, May 8

Registration 7:00 AM-5:30 PM Room:Society Hill Ballroom Foyer

Welcome Remarks 8:00 AM-8:15 AM Room:Society Hill Ballroom B,C,D,E Sunday, May 8

IP1 Effective Behavior of Random Media: An Error Analysis

8:15 AM-9:00 AM

Room:Society Hill Ballroom B,C,D,E

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

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

IP2

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

9:00 AM-9:45 AM

Room:Society Hill Ballroom B,C,D,E

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

Mikko Haataja Princeton University, USA

Coffee Break



9:45 AM-10:15 AM Room:Hamilton Room

Sunday, May 8

MS1

Mathematical Crystallography I. Tilings, Packings, Graphs, and Other Discrete Models -Part I of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom B

For Part 2 see MS12

Tilings and graphs are among the many discrete models of crystals, quasicrystals, and other highly ordered structures. The model consists of many components of a few types designed to capture the physical and chemical constraints of the molecular building blocks of which the modeled crystal is composed. These models may be used in analyzing extant crystals and in crystal structure prediction and design.

Organizer: Gregory McColm University of South Florida, USA

Organizer: Mile Krajcevski University of South Florida, USA

Organizer: Jean-Guillaume Eon

Universidade Federal do Rio De Janeiro, Brazil

Organizer: Marjorie Senechal Smith College, USA

10:15-10:40 Auxetics and Spectrahedra

Ciprian S. Borcea, Rider University, USA; Ileana Streinu, Smith College, USA

10:45-11:10 On Algebraic and Geometric Properties of Hyperbolic Tilings

Ma. Louise N. de las Penas, Ateneo de Manila University, Philippines

11:15-11:40 Entanglement in 2-Periodic Coordination Networks

Davide M. Proserpio, Università Degli Studi de Milano; Eugeny Alexandrov and Vladislav Blatov, Samara State Aerospace University, Russia

11:45-12:10 Polyhedral Origami Ileana Streinu, Smith College, USA

Sunday, May 8

MS2

Defects and Patterns in Thin Elastic Structures - Part I of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom C

For Part 2 see MS13

The formation of defects and patterns in thin sheets is familiar; examples include the wrinkling of a sheet wrapping a piece of fruit, and the cracking or blistering of a layer of paint. The variety of patterns is great, and we are just beginning to understand and harness them. This is an area where physics, geometry, and the calculus of variations interact intensely, each providing both challenges and tools. The minisymposium embraces the area's interdisciplinary character, combining mathematics with mechanics, experiment with theory, and analysis with computing.

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

10:15-10:40 Mechanical Response and Geometrical Constraints in Folded Sheets

Christian Santangelo, University of Massachusetts, Amherst, USA

10:45-11:10 Symmetry Breaking in Indented Elastic Cones

Sergio Conti and Heiner Olbermann, University of Bonn, Germany; *Ian Tobasco*, Courant Institute of Mathematical Sciences, New York University, USA

11:15-11:40 Programming Shape: Tapping Braille, Folding Origami, Printing Flowers

L Mahadevan, Harvard University, USA

11:45-12:10 The Smectic Order of Wrinkles

Hillel Aharoni, Eleni Katifori, and Randall Kamien, University of Pennsylvania, USA

MS3

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part I of VI

10:15 AM-12:15 PM

Room:Society Hill Ballroom D

For Part 2 see MS14

Polycrystalline grain microstructures are ubiquitous among technologically important materials, such as most metals and ceramics. The control of microstructures through processing is crucial to improvement of material properties, such as strength, toughness and electrical conductivity. This minisymposium will focus on understanding and prediction of thermodynamics and kinetics of grain microstructures. The minisymposium will bring together experts from materials science and mathematics and will include talks that range from experiments and modeling to algorithm development and analysis.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Selim Esedoglu University of Michigan, USA

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Dana Zoellner Otto-von-Guericke University, Magdenburg, Germany

10:15-10:40 Dislocations, Trijunctions and Grain Boundary Motion

Kevin McReynolds and *Peter Voorhees*, Northwestern University, USA

10:45-11:10 Atomistic Simulations of Line Defects at Interfaces

Mark Asta, Rodrigo Freitas, and Tim Frolov, University of California, Berkeley, USA

11:15-11:40 Grain Growth in Alloys: Atomistic and Phase Field Perspectives

S. M. Foiles, Fadi Abdeljawad, and Christopher O'Brien, Sandia National Laboratories, USA

11:45-12:10 Novel Application of Potts Model for Grain Growth During Welding using SPPARKS

John A. Mitchell and Veena Tikare, Sandia National Laboratories, USA

Sunday, May 8

MS4

Mathematics and Algorithms for Ground State Electronic Structure Theory -Part I of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom E

For Part 2 see MS15

Electronic structure theory and first principle calculations are among the most challenging and computationally demanding science and engineering problems. This minisymposium aims at presenting and discussing new developments of mathematical analysis and numerical methods for achieving ever higher level of accuracy and efficiency in ground state electronic structure theory. We bring together experts on electronic structure theory, which include not only mathematicians, but also physicists working actively in the field.

Organizer: Lin Lin University of California, Berkeley and Lawrence Berkeley National Laboratory, USA

Organizer: Jianfeng Lu Duke University, USA

Organizer: Gero Friesecke Technische Universität München, Germany

10:15-10:40 Mathematical Modeling of Multilayer 2D Materials

Eric Cances, Ecole des Ponts and Inria, France

10:45-11:10 Computing the Response Functions of Disordered Solids *Emil Prodan*, Yeshiva University, USA

11:15-11:40 A QM/MM Model for Material Interfaces

Xiantao Li, Pennsylvania State University, USA

11:45-12:10 Fast Algorithms for Localization of Kohn-Sham Orbitals Anil Damle, Stanford University, USA

15

Sunday, May 8

MS5

Complex Analysis, Optimization, and Herglotz Functions in Passive Electromagnetics and Composite Media -Part I of IV

10:15 AM-11:45 PM

Room:Society Hill Ballroom A1

For Part 2 see MS16

The aim of this minisymposium is to bring together a diverse group of researchers from mathematics, engineering, and physics that, although working on seemingly distinct topics, use similar tools from complex analysis or optimization theory in which Herglotz or Stieltjes functions are important. This minisymposium will help bring new insights and advancements in the theory of Herglotz functions and its applications by highlighting progress and challenges in the areas of multivariate complex analysis, electromagnetics, and the theory of composites. Topics include Herglotz functions, passive systems, complex analysis, optimization theory, dispersion relations, sum rules, bounds, and applications in electromagnetics and composites.

Organizer: Maxence Cassier University of Utah, USA

Organizer: Graeme W. Milton University of Utah, USA

Organizer: Mihai Putinar University of California, Santa Barbara, USA and Newcastle University, United Kingdom

Organizer: Aaron T. Welters Florida Institute of Technology, USA

10:15-10:40 Bounds on the Transient Response of Composites and Bodies *Graeme Milton*, University of Utah,

USA; Ornella Mattei, University of Brescia, Italy

10:45-11:10 The Spectrum of Composite Media in Two Dimensions and Energy Harvesting

Ross McPhedran, The University of Sydney, Australia

11:15-11:40 Generalized Wannier Functions

Emil Prodan, Yeshiva University, USA

Sunday, May 8

MS6

Computational Techniques for Multiscale Materials Modeling - Part I of III

10:15 AM-12:15 PM

Room:Society Hill Ballroom A2

For Part 2 see MS17

Emerging problems in micromechanical systems require modeling and computational effort across various physical scales. In this minisymposium we bring together an interdisciplinary group of researchers to focus on new developments in the analysis and simulations of complex material behavior, analytical and computational tools for the model reduction of atomiclevel descriptions and the mathematical foundations of multiscale modeling.

Organizer: Zhijian Yang Wuhan University, China

Organizer: Carlos Garcia Cervera University of California, Santa Barbara, USA

Organizer: Xiantao Li Pennsylvania State University, USA

Organizer: Pingbing Ming Chinese Academy of Sciences, China

10:15-10:40 Algorithms for Weighted (Anisotropic) Mean Curvature Motion of Networks

Selim Esedoglu, University of Michigan, USA

10:45-11:10 The String Method for Saddle Points Search

Weiqing Ren, National University of Singapore and IHPC, Singapore

11:15-11:40 Solitary Waves in Two Dimensional Lattices

Liping Liu, Rutgers University, USA

11:45-12:10 Density Functional Perturbation Theory for Large Systems *Lin Lin*, University of California,

Berkeley and Lawrence Berkeley National Laboratory, USA; Ze Xu, University of California, Berkeley, USA; Lexing Ying, Stanford University, USA

MS7

Modeling Mechanical Response in Disordered and Structurally Complex Materials Systems -Part I of IV

10:15 AM-12:15 PM

Room:Cook

For Part 2 see MS18

We propose a minisymposium exploring approaches to the quantification of microstructure with an eye to modeling mechanical response in materials that exhibit disorder and structural complexity. Examples of such systems include glasses, granular media, colloids, and biological systems. Many interesting interconnections can be drawn between these including incompatible embedded metrics that lead to residual stresses, poorly characterized structures that accommodate plasticity and flow, and a need to account for how forces are generated, accommodated and distributed. This minisymposium will bring together materials scientists, physicists, mathematicians and engineers to examine these problems from multiple overlapping perspectives.

Organizer: Michael L. Falk Johns Hopkins University, USA

Organizer: Timothy J. Atherton *Tufts University, USA*

10:15-10:40 Strain Localization and Fracture in Metallic Glass

Chris H. Rycroft, Harvard University, USA

10:45-11:10 Direct Measurements of Transformation Barriers in Glasses

Sylvain Patinet and Damien Vandembroucq, École Supérieure de Physique et de Chimie Industrielles, France; *Michael L. Falk*, Johns Hopkins University, USA

11:15-11:40 Softness: A Structural Approach to Failure or Relaxation in Disordered Systems

Andrea Liu, University of Pennsylvania, USA

11:45-12:10 Critical Scaling with Strain Rate in Overdamped Sheared Disordered Solids

Joel T. Clemmer and Mark Robbins, Johns Hopkins University, USA

Sunday, May 8

MS8

Modeling, Analysis and Simulation of Bio/Complex Fluids - Part I of III

10:15 AM-12:15 PM

Room:Flower

For Part 2 see MS19

Complex fluids are materials with a complicated microstructure, which can exhibit both viscous and elastic behaviors, for example polymer and surfactant 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, for example elastic instabilities such as shear banding, requiring detailed modeling combined with intricate analytic and simulation methods. The goal of this minisymposium is to bring together mathematicians and practitioners in the area to advance the subject through discussion and collaboration.

Organizer: Michael Cromer Rochester Institute of Technology, USA

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

10:15-10:40 Transient Shear Banding and the Two-Fluid Rolie-Poly Model

Michael Cromer, Rochester Institute of Technology, USA

10:45-11:10 Modeling Thixotropic Yield Stress Fluids As a Singular Limit of Viscoelasticity

Michael Renardy and Taige Wang, Virginia Tech, USA

11:15-11:40 Shear Banding in Entangled Polymeric Fluids and the Origin and Role of Spatially Inhomogeneous Dynamics

Elian Masnada and *Peter Olmsted*, Georgetown University, USA

11:45-12:10 Writhe and Mutual Entanglement Combine to Give the Entanglement Length

Eleni Panagiotou, University of California, Santa Barbara, USA; Martin Kroeger, ETH Zürich, Switzerland; Kenneth Millett, University of California, Santa Barbara, USA

MS9

Mesoscale Modeling of Non-Equilibrium Assembly, Transport, and Reaction Processes - Part I of III

10:15 AM-12:15 PM

Room:Bromley

For Part 2 see MS20

The mesoscale regime is where discrete atomistic-level descriptions of complex materials and processes transition to macroscopic continuum descriptions. Often features on this length scale provide the functionality, and their description generally includes heterogeneity and fluctuations absent in macroscopic treatments. Reliable formulations are required to enable systematic coarse-graining of deterministic and stochastic atomistic descriptions while retaining certain microscopic features, and may involve, e.g., non-equilibrium statistical mechanics, stochastic PDE's, generalized hydrodynamic formulations. This minisymposium will focus on non-equilibrium systems and processes: self-assembly and growth; transport and reaction in complex environments; etc., and development of related diverse modeling approaches.

Organizer: Jim W. Evans Ames Laboratory USDOE and Iowa State University, USA

Organizer: Petr Plechac University of Delaware, USA

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

10:15-10:40 Coarse-Grained Mesoscale Modeling for Deposition-Diffusion and Reaction-Diffusion Systems

James Evans, Ames Laboratory USDOE, USA; Tiago de Oliveira, Yong Han, Da-Jiang Liu, and Andres Garcia, Iowa State University, USA

10:45-11:10 Multiscale Modeling of Nanocrystal Growth in Solution

Kristen Fichthorn, Pennsylvania State University, USA

11:15-11:40 Shape-Based Modeling of the Self-Assembly Processes *Michael Engel*, University of Michigan, USA

11:45-12:10 Stratification of Markov Processes for Rare Event Simulation Jonathan Weare, University of Chicago, USA

Sunday, May 8

Quantifying Uncertainty and Stochasticity in Material Modeling - Part I of II

10:15 AM-12:15 PM

Room:Claypoole

For Part 2 see MS21

Over the past few decades, mathematical modelings as well as simulation tools have greatly enhanced the study of materials. However, deterministic approaches are often pushed to their limit, and the uncertainty in the models is often inevitable due to the intrinsic stochasticity of the materials. Uncertainty quantification (UQ) enters as a valuable tool that addresses issues on uncertainty propagation, optimal sampling, rare events, etc. This minisymposium aims at bringing researchers to discuss recent developments on UQ methods for material sciences that helps to understand the effect of uncertainty and stochasticity in material modeling including model calibration, material failure, transition paths.

Organizer: Huan Lei Pacific Northwest National Laboratory, USA

Organizer: Xiu Yang Pacific Northwest National Laboratory, USA

Organizer: Jing Li Pacific Northwest National Laboratory, USA

10:15-10:40 Discovery of Metastable and Transition States Using the Concurrent Adaptive Sampling Method

Surl-Hee Ahn and Eric F. Darve, Stanford University, USA

MS10 Quantifying Uncertainty and Stochasticity in Material Modeling - Part I of II

10:15 AM-12:15 PM

Room: Claypoole

continued

10:45-11:10 Data-Driven Parameterization of Memory Kernel in the Generalized Langevin Equation

Huan Lei and Nathan Baker, Pacific Northwest National Laboratory, USA; Xiantao Li, Pennsylvania State University, USA

11:15-11:40 Efficient Failure Probability Calculation Through Mesh Refinement

Jing Li and Panos Stinis, Pacific Northwest National Laboratory, USA

11:45-12:10 Bayesian Inference Using Gaussian Process Metamodel in Biomechanical Imaging

Assimina A. Pelegri and *Colin Cui*, Rutgers University, USA; Xiaodong Zhao, J.P. Morgan, USA

Sunday, May 8

MS11

Modern Aspects of Homogenization - Part I of III 10:15 AM-12:15 PM

Room:Frampton

For Part 2 see MS22

Homogenization can be used to rigorously derive effective descriptions for a broad variety of models featuring microstructure. In recent developments challenging aspects are discussed such as the quantification and identification of effects generated by disorder and noise, the treatment of nonlinearities, degeneracy and highcontrast. In this minisymposium we explore advances on the different frontiers of homogenization theory with the aim to encourage discussion and exchange of ideas. Specific topics include various aspects of stochastic homogenization, homogenization of nonlinear evolution, high-contrast homogenization, and applications to materials modelling.

Organizer: Stefan Neukamm Technische Universität Dresden, Germany

10:15-10:40 Stochastic Homogenization and the Random Conductance Model *Marek Biskup*, University of California, Los Angeles, USA

10:45-11:10 A Quantitative Two-Scale Expansion in Stochastic Homogenization

Stefan Neukamm, Technische Universität Dresden, Germany; Felix Otto, Max Planck Institute for Mathematics in the Sciences, Germany; Antoine Gloria, Université Libre de Bruxelles, Belgium

11:15-11:40 Eigenvalue Fluctuations for Lattice Anderson Hamiltonians

Ryoki Fukushima, Kyoto University, Japan; Marek Biskup, University of California, Los Angeles, USA; Wolfgang Koenig, Weierstrass Institute for Applied Analysis and Stochastics, Germany

11:45-12:10 Homogenization of Quasiperiodic Constitutive Relations

Niklas Wellander, Swedish Defense Research Agency, Sweden; Sébastien Guenneau, Institut Fresnel, France; Elena Cherkaev, University of Utah, USA Sunday, May 8 Lunch Break 12:15 PM-1:30 PM Attendees on their own

IP3

Topology and Geometry of Dislocation Networks under Extreme Straining

1:30 PM-2:15 PM

Room:Society Hill Ballroom B,C,D,E

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

Vasily Bulatov

Lawrence Livermore National Laboratory, USA

Intermission

2:15 PM-2:30 PM

MS12

Mathematical Crystallography II. Polyhedra, Cluster Models, and Assembly - Part II of IV

2:30 PM-4:30 PM

Room:Society Hill Ballroom B

For Part 1 see MS1 For Part 3 see MS23

Assembled and growing crystals, quasicrystals, and other highly ordered structures may be modeled using polyhedra and polytopes, Delaunay sets, complexes and clusters, and similar structures. While convex polyhedra have long used as tiles in representing periodic structures, generalized crystallography requires more generalized structures.

Organizer: Gregory McColm University of South Florida, USA

Organizer: Mile Krajcevski University of South Florida, USA

Organizer: Jean-Guillaume Eon Universidade Federal do Rio De Janeiro, Brazil

Organizer: Marjorie Senechal Smith College, USA

2:30-2:55 Algorithmic Self-Assembly and Self-Similar Structures

Natasha Jonoska, University of South Florida, USA

3:00-3:25 The Statistical Mechanics of Singular Sphere Packings

Miranda Holmes-Cerfon, Courant Institute of Mathematical Sciences, New York University, USA; Yoav Kallus, Santa Fe Institute, USA

3:30-3:55 What Role for Entropy in Stability and Growth of Quasicrystals?

Jean Taylor, Courant Institute of Mathematical Sciences, New York University, USA

4:00-4:25 Clusters of Polyhedra in Spherical Confinement

Erin G. Teich and Greg Van Anders, University of Michigan, USA; Daphne Klotsa, University of Michigan and University of North Carolina, USA; Julia Dshemuchadse and Sharon C. Glotzer, University of Michigan, USA

Sunday, May 8

MS13

Defects and Patterns in Thin Elastic Structures - Part II of IV

2:30 PM-4:30 PM

Room:Society Hill Ballroom C

For Part 1 see MS2 For Part 3 see MS24

The formation of defects and patterns in thin sheets is familiar; examples include the wrinkling of a sheet wrapping a piece of fruit, and the cracking or blistering of a layer of paint. The variety of patterns is great, and we are just beginning to understand and harness them. This is an area where physics, geometry, and the calculus of variations interact intensely, each providing both challenges and tools. The minisymposium embraces the area's interdisciplinary character, combining mathematics with mechanics, experiment with theory, and analysis with computing.

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

2:30-2:55 Non-Developable Isometries in Elastic Sheets

Benny Davidovitch, University of Massachusetts, Amherst, USA

3:00-3:25 Geometric Defects in Thin Elastic Structures

Shankar C. Venkataramani and Toby Shearman, University of Arizona, USA; John A. Gemmer, Brown University, USA

3:30-3:55 Wrinkling Reveals New Isometries of Elastic Sheets and Shells

Dominic Vella and Matteo Taffetani, University of Oxford, United Kingdom; Benny Davidovitch, University of Massachusetts, Amherst, USA

4:00-4:25 Regularizing Rigidifying Curves to Understand the Low-Energy Deformations of Thin Shells

Salem H. Al Mosleh and Christian Santangelo, University of Massachusetts, Amherst, USA

Sunday, May 8

MS14

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part II of VI

2:30 PM-4:30 PM

Room:Society Hill Ballroom D

For Part 1 see MS3 For Part 3 see MS25

Polycrystalline grain microstructures are ubiquitous among technologically important materials, such as most metals and ceramics. The control of microstructures through processing is crucial to improvement of material properties, such as strength, toughness and electrical conductivity. This minisymposium will focus on understanding and prediction of thermodynamics and kinetics of grain microstructures. The minisymposium will bring together experts from materials science and mathematics and will include talks that range from experiments and modeling to algorithm development and analysis.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Selim Esedoglu University of Michigan, USA

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Dana Zoellner Otto-von-Guericke University, Magdenburg, Germany

2:30-2:55 Graph Kernel Approaches to the Transgranular Network

Elizabeth Holm, Brian DeCost, and Anika Mangel, Carnegie Mellon University, USA

3:00-3:25 Coupled Modeling of Deformation and Recrystallization of Texture in Uranium

Marko Knezevic, University of New Hampshire, USA

MS14

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part II of VI

2:30 PM-4:30 PM

Room:Society Hill Ballroom D

continued

3:30-3:55 Recent Advances in the Simulation of Grain Boundary Migration and Related Phenomena: From the Atomistic to the Mesoscopic Scale

Luis Barrales-Mora, Dmitri A. Molodov, Markus Kühbach, and Christian Mießen, RWTH Aachen University, Germany

4:00-4:25 Recent Advances in the Full Field Modeling of Recrystallization and Grain Growth Using the Level Set Approach

Marc Bernacki, Benjamin Scholtes, and Nathalie Bozzolo, Mines ParisTech, France

Sunday, May 8

MS15

Mathematics and Algorithms for Ground State Electronic Structure Theory - Part II of IV

2:30 PM-4:30 PM

Room:Society Hill Ballroom E

For Part 1 see MS4 For Part 3 see MS26

Electronic structure theory and first principle calculations are among the most challenging and computationally demanding science and engineering problems. This minisymposium aims at presenting and discussing new developments of mathematical analysis and numerical methods for achieving ever higher level of accuracy and efficiency in ground state electronic structure theory. We bring together experts on electronic structure theory, which include not only mathematicians, but also physicists working actively in the field.

Organizer: Lin Lin University of California, Berkeley and Lawrence Berkeley National Laboratory, USA

Organizer: Jianfeng Lu Duke University, USA

Organizer: Gero Friesecke Technische Universität München, Germany

2:30-2:55 Acceleration of Hybrid Density Functional Computations Using Recursive Subspace Bisection

Francois Gygi, University of California, Davis, USA

3:00-3:25 A Posteriori Quantification of Model/discretization/solution Method Errors for Electronic Structure Calculations

Yvon Maday, Université Pierre et Marie Curie, France and Brown University, USA

3:30-3:55 Chebyshev Filtered Subspace Iterations Within the Framework of Discontinuous Galerkin Density Functional Theory for Large Scale Abinitio Simulations

Amartya S. Banerjee and Wei Hu, Lawrence Berkeley National Laboratory, USA; Lin Lin, University of California, Berkeley and Lawrence Berkeley National Laboratory, USA; Chao Yang, Lawrence Berkeley National Laboratory, USA; John Pask, Lawrence Livermore National Laboratory, USA

4:00-4:25 Improving Density Functional Theory for Warm Dense Matter

Aurora Pribram-Jones, University of California, Irvine, USA

MS16

Complex Analysis, Optimization, and Herglotz Functions in Passive Electromagnetics and Composite Media -Part II of IV

2:30 PM-4:00 PM

Room:Society Hill Ballroom A1

For Part 1 see MS5 For Part 3 see MS27

The aim of this minisymposium is to bring together a diverse group of researchers from mathematics, engineering, and physics that, although working on seemingly distinct topics, use similar tools from complex analysis or optimization theory in which Herglotz or Stieltjes functions are important. This minisymposium will help bring new insights and advancements in the theory of Herglotz functions and its applications by highlighting progress and challenges in the areas of multivariate complex analysis, electromagnetics, and the theory of composites. Topics include Herglotz functions, passive systems, complex analysis, optimization theory, dispersion relations, sum rules, bounds, and applications in electromagnetics and composites.

Organizer: Maxence Cassier University of Utah, USA

Organizer: Graeme W. Milton University of Utah, USA

Organizer: Mihai Putinar University of California, Santa Barbara, USA and Newcastle University, United Kingdom

Organizer: Aaron T. Welters Florida Institute of Technology, USA

2:30-2:55 Bounds on Stieltjes Functions and Their Applications to Passive Cloaking

Maxence Cassier and Graeme Milton, University of Utah, USA

3:00-3:25 Complex Analysis and Herglotz Functions in the Mathematics of Sea Ice

Kenneth Golden, University of Utah, USA

3:30-3:55 Herglotz Functions and Sum Rules for Passive Systems

Mats Gustafsson, Lund University, Sweden

Sunday, May 8

Computational Techniques for Multiscale Materials Modeling - Part II of III

2:30 PM-4:30 PM

Room:Society Hill Ballroom A2

For Part 1 see MS6 For Part 3 see MS28

Emerging problems in micromechanical systems require modeling and computational effort across various physical scales. In this minisymposium we bring together an interdisciplinary group of researchers to focus on new developments in the analysis and simulations of complex material behavior, analytical and computational tools for the model reduction of atomic-level descriptions and the mathematical foundations of multiscale modeling.

Organizer: Zhijian Yang Wuhan University, China

USA

Organizer: Carlos Garcia Cervera University of California, Santa Barbara,

Organizer: Xiantao Li Pennsylvania State University, USA

Organizer: Pingbing Ming Chinese Academy of Sciences, China

2:30-2:55 Modelling and Simulation of Magnetic Fluids

Hector D. Ceniceros, University of California, Santa Barbara, USA

3:00-3:25 Traction Boundary Conditions for Molecular Static Simulations *Jianfeng Lu*, Duke University, USA

3:30-3:55 Recent Development of Numerical Methods on Finding Saddle Point and Minimum Energy Path Lei Zhang, Peking University, China

4:00-4:25 A Coupling Strategy for Nonlocal and Local Models with Mixed Volume Constraints and Boundary Conditions *Marta D'Elia*, Sandia National

Laboratories, USA

MS18

Modeling Mechanical Response in Disordered and Structurally Complex Materials Systems -Part II of IV

2:30 PM-4:30 PM

Room:Cook

For Part 1 see MS7 For Part 3 see MS29

We propose a minisymposium exploring approaches to the quantification of microstructure with an eye to modeling mechanical response in materials that exhibit disorder and structural complexity. Examples of such systems include glasses, granular media, colloids, and biological systems. Many interesting interconnections can be drawn between these including incompatible embedded metrics that lead to residual stresses, poorly characterized structures that accommodate plasticity and flow, and a need to account for how forces are generated, accommodated and distributed. This minisymposium will bring together materials scientists, physicists, mathematicians and engineers to examine these problems from multiple overlapping perspectives.

Organizer: Michael L. Falk Johns Hopkins University, USA

Organizer: Timothy J. Atherton *Tufts University, USA*

2:30-2:55 Universal Slip Statistics: From Nanocrystals to Earthquakes

Karin Dahmen, University of Illinois, USA

3:00-3:25 Inter-Particle Force Inference in Opaque Granular Materials Imaged Using X-Ray Tomography and Diffraction

Ryan C. Hurley, Lawrence Livermore National Laboratory and Johns Hopkins University, USA; Stephen Hall, Lund University, Sweden; Jose Andrade, California Institute of Technology, USA; Jonathan Wright, European Synchrotron Radiation Facility, France

3:30-3:55 How Do Hard-Sphere Colloidal Glasses Respond to Deformation?

Katharine E. Jensen, Yale University, USA

4:00-4:25 Jammed Packings on Arrested Emulsion Droplets

Christopher J. Burke and Timothy J. Atherton, Tufts University, USA

Sunday, May 8

MS19

Modeling, Analysis and Simulation of Bio/Complex Fluids - Part II of III

2:30 PM-4:30 PM

Room:Flower

For Part 1 see MS8 For Part 3 see MS30

Complex fluids are materials with a complicated microstructure, which can exhibit both viscous and elastic behaviors, for example polymer and surfactant 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, for example elastic instabilities such as shear banding, requiring detailed modeling combined with intricate analytic and simulation methods. The goal of this minisymposium is to bring together mathematicians and practitioners in the area to advance the subject through discussion and collaboration.

Organizer: Michael Cromer Rochester Institute of Technology, USA

Organizer: Lin Zhou New York City College of Technology, USA 2:30-2:55 Deformation and Yielding in Soft Solids

Emanuela Del Gado, Georgetown University, USA

3:00-3:25 Mesoscopic Modelling of Viscoelastic Properties of Micellar Solutions

Weizhong Zou and Ronald Larson, University of Michigan, Ann Arbor, USA; Xueming Tang, University of Michigan, USA; Mike Weaver and Peter Koening, Procter & Gamble, USA

3:30-3:55 Mesoscopic Modeling of Networked Fluids

Lin Zhou, New York City College of Technology, USA; L. Pamela Cook, University of Delaware, USA

4:00-4:25 Simple Approach of Stress Diffusion in Shear Banding

Elian Masnada and Peter Olmsted, Georgetown University, USA

MS20

Mesoscale Modeling of Non-Equilibrium Assembly, Transport, and Reaction Processes - Part II of III

2:30 PM-4:30 PM

Room:Bromley

For Part 1 see MS9 For Part 3 see MS31

The mesoscale regime is where discrete atomistic-level descriptions of complex materials and processes transition to macroscopic continuum descriptions. Often features on this length scale provide the functionality, and their description generally includes heterogeneity and fluctuations absent in macroscopic treatments. Reliable formulations are required to enable systematic coarse-graining of deterministic and stochastic atomistic descriptions while retaining certain microscopic features, and may involve, e.g., non-equilibrium statistical mechanics, stochastic PDE's, generalized hydrodynamic formulations. This minisymposium will focus on non-equilibrium systems and processes: self-assembly and growth; transport and reaction in complex environments; etc., and development of related diverse modeling approaches.

Organizer: Jim W. Evans Ames Laboratory USDOE and Iowa State University, USA

Organizer: Petr Plechac University of Delaware, USA

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

2:30-2:55 Information-Theoretic Tools for Coarse-Graining of Non-Equilibrium Systems

Markos A. Katsoulakis, University of Massachusetts, Amherst, USA; Petr Plechac, University of Delaware, USA

3:00-3:25 Fronts and Patterns in Surface Reaction-Diffusion Systems from Molecular-Level Modeling: CO Oxidation on Metals

Da-Jiang Liu, Ames Laboratory USDOE, USA; Jim W. Evans, Ames Laboratory USDOE and Iowa State University, USA

3:30-3:55 First Principles Prediction of Optimal Catalyst Active Site

Dion Vlachos, University of Delaware, USA

4:00-4:25 Mesoscale Model of Reaction Front Propagation in Heterogeneous Condensed Systems

Yuriy Gulak and *Alberto Cuitino*, Rutgers University, USA

Sunday, May 8

MS21

Quantifying Uncertainty and Stochasticity in Material Modeling - Part II of II

2:30 PM-5:00 PM

Room:Claypoole

For Part 1 see MS10 For Part 3 see MS32

Over the past few decades. mathematical modelings as well as simulation tools have greatly enhanced the study of materials. However, deterministic approaches are often pushed to their limit, and the uncertainty in the models is often inevitable due to the intrinsic stochasticity of the materials. Uncertainty quantification (UQ) enters as a valuable tool that addresses issues on uncertainty propagation, optimal sampling, rare events, etc. This minisymposium aims at bringing researchers to discuss recent developments on UQ methods for material sciences that helps to understand the effect of uncertainty and stochasticity in material modeling including model calibration, material failure, transition paths.

Organizer: Huan Lei Pacific Northwest National Laboratory, USA

Organizer: Xiu Yang Pacific Northwest National Laboratory, USA

Organizer: Jing Li Pacific Northwest National Laboratory, USA

2:30-2:55 Polymer Looping: Kinetics and Mean First Passage Time

Panos Stinis, Pacific Northwest National Laboratory, USA

3:00-3:25 Adaptive Minimum Action Method for Nongradient Systems *Xiaoliang Wan*, Louisiana State

University, USA

continued on next page

MS21

Quantifying Uncertainty and Stochasticity in Material Modeling - Part II of II

2:30 PM-5:00 PM

Room:Claypoole

continued

3:30-3:55 A Coarse-Grained and Time Accelerated Modeling for Protein Unfolding Dynamics

Xingjie Li, University of North Carolina, Charlotte, USA; Mingge Deng and George E. Karniadakis, Brown University, USA; Jianfeng Lu, Duke University, USA; Xiu Yang, Pacific Northwest National Laboratory, USA

4:00-4:25 Sensitivity Analysis of the Reaxff Potential Parameter-Space

Efrain Hernandez, Shawn Coleman, and Mark Tschopp, U.S. Army Research Laboratory, USA

4:30-4:55 Predictive Coarse-Graining

Markus Schöberl, Technische Universität München, Germany; Nicholas Zabaras, University of Warwick, United Kingdom; Phaedon S. Koutsourelakis, Technische Universität München, Germany Sunday, May 8

MS22

Modern Aspects of Homogenization - Part II of III 2:30 PM-4:00 PM

Room:Frampton

For Part 1 see MS11 For Part 3 see MS33

Homogenization can be used to rigorously derive effective descriptions for a broad variety of models featuring microstructure. In recent developments challenging aspects are discussed such as the quantification and identification of effects generated by disorder and noise, the treatment of nonlinearities, degeneracy and high-contrast. In this minisymposium we explore advances on the different frontiers of homogenization theory with the aim to encourage discussion and exchange of ideas. Specific topics include various aspects of stochastic homogenization, homogenization of nonlinear evolution, high-contrast homogenization, and applications to materials modelling.

Organizer: Stefan Neukamm Technische Universität Dresden, Germany

2:30-2:55 Homogenisation for Mean Field Games

Nicolas Dirr, Cardiff University, United Kingdom

3:00-3:25 A Multiscale Damage Model in the Context of Evolutionary Gamma-Convergence

Dorothee Knees, University of Kassel, Germany

3:30-3:55 Homogenization in Fractional Elasticity

Marcus Waurick, University of Bath, United Kingdom

Coffee Break

4:30 PM-5:00 PM Room:Hamilton Room



Sunday, May 8

MS23

Mathematical Crystallography III. Groups, Lattices, Spaces and Superspaces - Part III of IV 5:00 PM-7:00 PM

Room:Society Hill Ballroom B

For Part 2 see MS12 For Part 4 see MS34

Models of crystals, quasicrystals, and other highly ordered structures often have underlying regularities or symmetries expressible by some kind of group structure. The geometric lattice, the resulting lattice group, and its symmetry group may be derived from a (periodic) discrete model of a crystal structure or from higher dimensional lattices.

Organizer: Gregory McColm University of South Florida, USA

Organizer: Mile Krajcevski University of South Florida, USA

Organizer: Jean-Guillaume Eon Universidade Federal do Rio De Janeiro, Brazil

Organizer: Marjorie Senechal Smith College, USA

5:00-5:25 Materials Studies by the Bilbao Crystallographic Server

Mois I. Aroyo, J.Manuel Perez-Mato, Luis Elcoro, Samuel Gallego, and Gemma de la Flor, Universidad del País Vasco, Spain; Emre Tasci, Hacettepe Universýty, Turkey; Gotzon Madariaga, Universidad del País Vasco, Spain

5:30-5:55 The 12 Spheres Problem

Jeffrey Lagarias, University of Michigan, USA; Robert Kusner, University of Massachusetts, Amherst, USA; Woden Kusner, Graz University of Technology, Austria; Senya Shlosman, Aix-Marseille University and Universite de Toulon, France

6:00-6:25 Applications of Groupoids to the Description and Interpretation of Crystal Structures: The Example of Pyxorenes

Massimo Nespolo, Université de Lorraine, France; Mois I. Aroyo, Universidad del País Vasco, Spain

6:30-6:55 Recognizing the Lattice Type to Which a Unit Cell (almost) Belongs

Bernd Souvignier, Radboud University, The Netherlands

Sunday, May 8

MS24

Defects and Patterns in Thin Elastic Structures -Part III of IV

5:00 PM-6:30 PM

Room:Society Hill Ballroom C

For Part 2 see MS13 For Part 4 see MS35

The formation of defects and patterns in thin sheets is familiar; examples include the wrinkling of a sheet wrapping a piece of fruit, and the cracking or blistering of a layer of paint. The variety of patterns is great, and we are just beginning to understand and harness them. This is an area where physics, geometry, and the calculus of variations interact intensely, each providing both challenges and tools. The minisymposium embraces the area's interdisciplinary character, combining mathematics with mechanics. experiment with theory, and analysis with computing.

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

5:00-5:25 Self-Similar Folding Patterns in Partially Delaminated Thin Films

David P. Bourne, Durham University, United Kingdom; Sergio Conti and Stefan Mueller, University of Bonn, Germany

5:30-5:55 Brittle Linearly Elastic Thin Films

J.-F. Babadjian, Laboratoire Jacques-Louis Lions and Université Paris
6, France; *Duvan Henao*, Pontificia Universidad Católica de Chile, Chile

6:00-6:25 A Variational Model for Fracture and Debonding of Thin Films Under In-Plane Loadings

Andrés A León Baldelli, University of Oxford, United Kingdom; J.-F. Babadjian, Laboratoire Jacques-Louis Lions and Université Paris 6, France; B. Bourdin, Louisiana State University, USA; D. Henao, Pontificia Universidad Católica de Chile, Chile; C. Maurini, Institut Jean le Rond d'Alembert, France

Sunday, May 8

MS25

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part III of VI

5:00 PM-7:00 PM

Room:Society Hill Ballroom D

For Part 2 see MS14 For Part 4 see MS36

Polycrystalline grain microstructures are ubiquitous among technologically important materials, such as most metals and ceramics. The control of microstructures through processing is crucial to improvement of material properties, such as strength, toughness and electrical conductivity. This minisymposium will focus on understanding and prediction of thermodynamics and kinetics of grain microstructures. The minisymposium will bring together experts from materials science and mathematics and will include talks that range from experiments and modeling to algorithm development and analysis.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Selim Esedoglu University of Michigan, USA

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Dana Zoellner Otto-von-Guericke University, Magdenburg, Germany

5:00-5:25 Grain Growth in Metallic Films: Simulations and Experiments Katayun Barmak, Columbia University,

USA

MS25

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part III of VI

5:00 PM-7:00 PM

continued

5:30-5:55 Growth of Grain Boundary Grooves by Anomalous Surface Diffusion

Alexander Nepomnyashchy and Mohammad Abu Hamed, Technion -Israel Institute of Technology, Israel

6:00-6:25 Surface Effects on Grain Boundary Migration in Thin Films

Amy Novick-Cohen, Technion - Israel Institute of Technology, Israel; John McCuan, Georgia Institute of Technology, USA; Arkady Vilenkin, Hebrew University of Jerusalem, Israel

6:30-6:55 Convergence of Thresholding Schemes for Mean-Curvature Motion

Tim Laux and Felix Otto, Max Planck Institute for Mathematics in the Sciences, Germany; Drew Swartz, Booz Allen Hamilton, USA

Sunday, May 8

MS26

Mathematics and Algorithms for Ground State Electronic Structure Theory -Part III of IV

5:00 PM-7:00 PM

Room:Society Hill Ballroom E

For Part 2 see MS15 For Part 4 see MS37

Electronic structure theory and first principle calculations are among the most challenging and computationally demanding science and engineering problems. This minisymposium aims at presenting and discussing new developments of mathematical analysis and numerical methods for achieving ever higher level of accuracy and efficiency in ground state electronic structure theory. We bring together experts on electronic structure theory, which include not only mathematicians, but also physicists working actively in the field.

Organizer: Lin Lin University of California, Berkeley and Lawrence Berkeley National Laboratory, USA

Organizer: Jianfeng Lu Duke University, USA

Organizer: Gero Friesecke Technische Universität München, Germany

5:00-5:25 Algorithms for Large-Scale All-Electron Density Functional Theory and Beyond

Volker Blum, Duke University, USA

5:30-5:55 The Flexibility of Daubechies Wavelets for Electronic Structure Calculations

Luigi Genovese, CEA, France

6:00-6:25 Large-Scale Real-Space All-Electron Kohn-Sham Density Functional Theory Calculations

Bikash Kanungo and *Vikram Gavini*, University of Michigan, USA

6:30-6:55 Fast Electronic Structure Calculation Methods for Studying Lowdimensional Nanomaterials

Chao Yang, Lawrence Berkeley National Laboratory, USA

Sunday, May 8

MS27

Complex Analysis, Optimization, and Herglotz Functions in Passive Electromagnetics and Composite Media -Part III of IV

5:00 PM-6:30 PM

Room:Society Hill Ballroom A1

For Part 2 see MS16 For Part 4 see MS38

The aim of this minisymposium is to bring together a diverse group of researchers from mathematics, engineering, and physics that, although working on seemingly distinct topics, use similar tools from complex analysis or optimization theory in which Herglotz or Stieltjes functions are important. This minisymposium will help bring new insights and advancements in the theory of Herglotz functions and its applications by highlighting progress and challenges in the areas of multivariate complex analysis, electromagnetics, and the theory of composites. Topics include Herglotz functions, passive systems, complex analysis, optimization theory, dispersion relations, sum rules, bounds, and applications in electromagnetics and composites.

Organizer: Maxence Cassier University of Utah, USA

Organizer: Graeme W. Milton University of Utah, USA

Organizer: Mihai Putinar University of California, Santa Barbara, USA and Newcastle University, United Kingdom

Organizer: Aaron T. Welters Florida Institute of Technology, USA

5:00-5:25 Analyticity of the Dirichletto-Neumann Map for Maxwell's Equations in Passive Composite Media

Aaron Welters, Florida Institute of Technology, USA; Maxence Cassier and Graeme W. Milton, University of Utah, USA

5:30-5:55 Matrix Pade Approximants of Stieltjes Functions

Elena Cherkaev, University of Utah, USA

6:00-6:25 Determination of Optimal Performance of Electromagnetic Devices Using Convex Optimization

Daniel Sjöberg, Lund University, Sweden

Sunday, May 8

MS28

Computational Techniques for Multiscale Materials Modeling - Part III of III

5:00 PM-7:00 PM

Room:Society Hill Ballroom A2

For Part 2 see MS17

Emerging problems in micromechanical systems require modeling and computational effort across various physical scales. In this minisymposium we bring together an interdisciplinary group of researchers to focus on new developments in the analysis and simulations of complex material behavior, analytical and computational tools for the model reduction of atomiclevel descriptions and the mathematical foundations of multiscale modeling.

Organizer: Zhijian Yang Wuhan University, China

Organizer: Carlos Garcia Cervera University of California, Santa Barbara, USA

Organizer: Xiantao Li Pennsylvania State University, USA

Organizer: Pingbing Ming Chinese Academy of Sciences, China

5:00-5:25 Variational Analysis of a Quasicontinuum Method

Anja Schlömerkemper, University of Würzburg, Germany; Mathias Schäffner, Technische Universität Dresden, Germany

5:30-5:55 Embedded Corrector Problem and Boundary Integral Methods for Stochastic Homogenization

Virginie Ehrlacher, CERMICS, France; Eric Cances, Ecole des Ponts and Inria, France; Benjamin Stamm, University of California, Berkeley, USA; Frederic Legoll, Ecole Nationale des Ponts et Chaussées, France 6:00-6:25 Simulations of Material Interface Problems Using Atomistic-Based Boundary Element Method

Xiaojie Wu, Pennsylvania State University, USA

6:30-6:55 Application of the Multiscale Micromorphic Molecular Dynamics for Nanoindentation of Silicon

Shingo Urata and Shaofan Li, University of California, Berkeley, USA

MS29

Modeling Mechanical Response in Disordered and Structurally Complex Materials Systems -Part III of IV

5:00 PM-7:00 PM

Room:Cook

For Part 2 see MS18 For Part 4 see MS40

We propose a minisymposium exploring approaches to the quantification of microstructure with an eye to modeling mechanical response in materials that exhibit disorder and structural complexity. Examples of such systems include glasses, granular media, colloids, and biological systems. Many interesting interconnections can be drawn between these including incompatible embedded metrics that lead to residual stresses, poorly characterized structures that accommodate plasticity and flow, and a need to account for how forces are generated, accommodated and distributed. This minisymposium will bring together materials scientists, physicists, mathematicians and engineers to examine these problems from multiple overlapping perspectives.

Organizer: Michael L. Falk Johns Hopkins University, USA

Organizer: Timothy J. Atherton *Tufts University, USA*

5:00-5:25 Arresting Relaxation in Pickering Emulsions

Timothy J. Atherton, Tufts University, USA

5:30-5:55 Shape Formation in Plates with Incompatible Pre-Strains

Marta Lewicka, University of Pittsburgh, USA

6:00-6:25 The Buckling-Fracture Transition in Non-Euclidean Plates

Eran Sharon, The Hebrew University, Israel

6:30-6:55 Homogenization of Defects: The Emergence of Torsion and Non-Metricity

Raz Kupferman, Hebrew University, Israel

Sunday, May 8

MS30

Modeling, Analysis and Simulation of Bio/Complex Fluids - Part III of III

5:00 PM-7:00 PM

Room:Flower

For Part 2 see MS19

Complex fluids are materials with a complicated microstructure, which can exhibit both viscous and elastic behaviors, for example polymer and surfactant 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, for example elastic instabilities such as shear banding, 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 Rochester Institute of Technology, USA

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

5:00-5:25 Mucus Microrheology as an Assay for Disease Progression and Drug Treatment

M. Gregory Forest, University of North Carolina at Chapel Hill, USA

5:30-5:55 A Stochastic Model of Lung Mucus Gel Networks

Erik Palmer, University of South Carolina, USA; M. Gregory Forest, University of North Carolina at Chapel Hill, USA; Paula A. Vasquez, University of South Carolina, USA

6:00-6:25 Modeling the Macroscopic Rheological Response of Mucin Gels Using Microscopic Polymer Network Considerations

Caroline Wagner, Brad Turner, Katharina Ribbeck, and Gareth H. McKinley, Massachusetts Institute of Technology, USA

6:30-6:55 A Multiscale Model for the Thixotropic Rheology of Colloidal Suspensions

Paul Mwasame, Antony N. Beris, and Norman Wagner, University of Delaware, USA

continued in next column

28

MS31

Mesoscale Modeling of Non-Equilibrium Assembly, Transport, and Reaction Processes - Part III of III

5:00 PM-7:00 PM

Room:Bromley

For Part 2 see MS20

The mesoscale regime is where discrete atomistic-level descriptions of complex materials and processes transition to macroscopic continuum descriptions. Often features on this length scale provide the functionality, and their description generally includes heterogeneity and fluctuations absent in macroscopic treatments. Reliable formulations are required to enable systematic coarse-graining of deterministic and stochastic atomistic descriptions while retaining certain microscopic features, and may involve, e.g., non-equilibrium statistical mechanics, stochastic PDE's, generalized hydrodynamic formulations. This minisymposium will focus on nonequilibrium systems and processes: self-assembly and growth; transport and reaction in complex environments; etc., and development of related diverse modeling approaches.

Organizer: Jim W. Evans Ames Laboratory USDOE and Iowa State University, USA

Organizer: Petr Plechac University of Delaware, USA

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

5:00-5:25 A Dynamic Phase-Field Model for Structural Transformations and Twinning: Regularized Interfaces with Transparent Prescription of Complex Kinetics and Nucleation

Kaushik Dayal, Carnegie Mellon University, USA 5:30-5:55 Mesoscale Modeling of Stress-Directed Compositional Patterning in Semiconductor Alloys *Talid Sinno*, University of Pennsylvania, USA

6:00-6:25 Mesoscopic Simulations of Lipid Membrane Remodeling

Aram Davtyan, University of Chicago, USA

6:30-6:55 Multiresolution of Molecular Dynamics in the Particle Domain

B. Chistopher Rinderspacher, U.S. Army Research Laboratory, USA

Sunday, May 8

MS32

Quantifying Uncertainty and Stochasticity in Material Modeling CANCELLED

5:00 PM-7:00 PM

Room:Claypoole

For Part 2 see MS21

Over the past few decades, mathematical modelings as well as simulation tools have greatly enhanced the study of materials. How ver deterministic approach are often pushed to their limit, and the uncertainty in the models is often inevitable due to the intrinsic stochasticity of the materials. Uncertainty quantification (UQ) enters as a valuable tool that addresses issues on uncertainty propagation, optimal sampling, rare events, etc. This minisymposium aims at bringing researchers to discuss recent developments on UQ methods for material sciences that helps to understand the effect of uncertainty and stochasticity in material modeling including model calibration, material failure, transition paths.

Organizer: Huan Lei Pacific Northwest National Laboratory, USA

Organizer: Xiu Yang Pacific Northwest National Laboratory, USA

Organizer: Jing Li Pacific Northwest National Laboratory, USA

MS33 Modern Aspects of Homogenization - Part III of III

5:00 PM-6:30 PM

Room:Frampton

For Part 2 see MS22

Homogenization can be used to rigorously derive effective descriptions for a broad variety of models featuring microstructure. In recent developments challenging aspects are discussed such as the quantification and identification of effects generated by disorder and noise, the treatment of nonlinearities, degeneracy and high-contrast. In this minisymposium we explore advances on the different frontiers of homogenization theory with the aim to encourage discussion and exchange of ideas. Specific topics include various aspects of stochastic homogenization, homogenization of nonlinear evolution, high-contrast homogenization, and applications to materials modelling.

Organizer: Stefan Neukamm Technische Universität Dresden, Germany

5:00-5:25 Norm-Resolvent Convergence of One-Dimensional High-Contrast Periodic Problems to a Kronig-Penney Dipole-Type Model

Kirill Cherednichenko, University of Bath, United Kingdom; Alexander Kiselev, National Pedagogical Dragomanov University, Ukraine

5:30-5:55 Effective Maxwell's Equations in a Geometry with Flat Split-Rings

Agnes Lamacz, Technische Universität Dortmund, Germany

6:00-6:25 Homogenization of Discrete Systems with Degenerated Growth

Mathias Schäffner and Stefan Neukamm, Technische Universität Dresden, Germany; Anja Schlömerkemper, University of Würzburg, Germany

Monday, May 9

Registration 7:30 AM-5:30 PM Room:Society Hill Ballroom Foyer

Remarks 8:00 AM-8:15 AM Room:Society Hill Ballroom B,C,D,E

IP4

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

8:15 AM-9:00 AM

Room:Society Hill Ballroom B,C,D,E

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

Carl E. Krill III Ulm University, Germany

Monday, May 9

IP5

Theory and Challenges for Microstructure Evolution 9:00 AM-9:45 AM

Room:Society Hill Ballroom B,C,D,E

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

David Kinderlehrer Carnegie Mellon University, USA

Coffee Break

9:45 AM-10:15 AM Room:Hamilton Room



MS34 Mathematical Crystallography

IV. Beyond Crystallography -

Part IV of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom B

For Part 3 see MS23

Some models of crystals, from periodic and aperiodic graphs to polytope complexes, may be generalized to encompass functional, hierarchical structures, and other highly regular structures in materials science and nanoscience.

Organizer: Gregory McColm University of South Florida, USA

Organizer: Mile Krajcevski University of South Florida, USA

Organizer: Jean-Guillaume Eon Universidade Federal do Rio De Janeiro, Brazil

Organizer: Marjorie Senechal *Smith College, USA*

10:15-10:40 Skeletal Polyhedral Complexes and Nets with High Symmetry

Egon Schulte, Northeastern University, USA

10:45-11:10 Molecular Packing Problems and Quotients of the Euclidean Group by Space Groups

Gregory Chirikjian, Johns Hopkins University, USA

11:15-11:40 Diffraction and Dynamical Spectra in Aperiodic Order

Uwe Grimm, The Open University, United Kingdom; Michael Baake, University of Bielefeld, Germany

11:45-12:10 Comparing Coincidence Rotations and Similarity Transformations of Lattices and Modules

Peter Zeiner, University of Bielefeld, Germany

Monday, May 9

MS35

Defects and Patterns in Thin Elastic Structures -Part IV of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom C

For Part 3 see MS24

The formation of defects and patterns in thin sheets is familiar; examples include the wrinkling of a sheet wrapping a piece of fruit, and the cracking or blistering of a layer of paint. The variety of patterns is great, and we are just beginning to understand and harness them. This is an area where physics, geometry, and the calculus of variations interact intensely, each providing both challenges and tools. The minisymposium embraces the area's interdisciplinary character, combining mathematics with mechanics, experiment with theory, and analysis with computing.

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

10:15-10:40 Gaussian Curvature as an Identifier of Shell Rigidity

Davit Harutyunyan, University of Utah, USA

10:45-11:10 Putting Patterns on Pollen

Maxim O. Lavrentovich, Eric Horsley, Asja Radja, Alison Sweeney, and Randall Kamien, University of Pennsylvania, USA

11:15-11:40 Isometric Immersions, Energy Minimization and Branch Points in Non-Euclidean Elastic Sheets

John A. Gemmer, Brown University, USA; Shankar C. Venkataramani, University of Arizona, USA; Eran Sharon, The Hebrew University, Israel; Toby Shearman, University of Arizona, USA

11:45-12:10 Metric Frustration Selects Morphology of Chiral Filament Bundles

Doug M. Hall, University of
Massachusetts, Amherst, USA; Isaac
R. Bruss, University of Michigan,
USA; *Gregory M. Grason*, University
of Massachusetts, Amherst, USA

Monday, May 9

MS36

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part IV of VI

10:15 AM-12:15 PM

Room:Society Hill Ballroom D

For Part 3 see MS25 For Part 5 see MS47

Polycrystalline grain microstructures are ubiquitous among technologically important materials, such as most metals and ceramics. The control of microstructures through processing is crucial to improvement of material properties, such as strength, toughness and electrical conductivity. This minisymposium will focus on understanding and prediction of thermodynamics and kinetics of grain microstructures. The minisymposium will bring together experts from materials science and mathematics and will include talks that range from experiments and modeling to algorithm development and analysis.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Selim Esedoglu University of Michigan, USA

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Dana Zoellner Otto-von-Guericke University, Magdenburg, Germany

10:15-10:40 A New Look on Scaling: The Envelope of Size Distributions in Ostwald Ripening and Grain Growth

Dana Zoellner and Peter Streitenberger, Otto-von-Guericke University, Magdenburg, Germany

MS36

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part IV of VI

10:15 AM-12:15 PM

Room:Society Hill Ballroom D continued

10:45-11:10 Grain Boundary Character Distribution and Mass Transport Paradigm

Yekaterina Epshteyn, University of Utah, USA

11:15-11:40 Kinetic Models for 2D Grain Growth

Govind Menon, Brown University, USA; Robert Pego, Carnegie Mellon University, USA; Joe Klobusicky, Geisinger Health Systems, USA

11:45-12:10 Stochastic Processes in Mesoscale Modeling of Polycrystals

Diego Torrejon and Maria Emelianenko, George Mason University, USA

Monday, May 9

MS37

Mathematics and Algorithms for Ground State Electronic Structure Theory - Part IV of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom E

For Part 3 see MS26

Electronic structure theory and first principle calculations are among the most challenging and computationally demanding science and engineering problems. This minisymposium aims at presenting and discussing new developments of mathematical analysis and numerical methods for achieving ever higher level of accuracy and efficiency in ground state electronic structure theory. We bring together experts on electronic structure theory, which include not only mathematicians, but also physicists working actively in the field.

Organizer: Lin Lin

University of California, Berkeley and Lawrence Berkeley National Laboratory, USA

Organizer: Jianfeng Lu Duke University, USA

Organizer: Gero Friesecke Technische Universität München, Germany

10:15-10:40 Tensor Networks and Related Representation for Electronic Schrodinger Equation

Reinhold Schneider, Technische Universität Berlin, Germany

10:45-11:10 Pair Densities in Density Functional Theory

Huajie Chen, University of Warwick, United Kingdom; Gero Friesecke, Technische Universität München, Germany

11:15-11:40 Spectral Gauss Quadrature Method with Subspace Interpolation for Kohn-Sham Density Functional Theory

Xin Cindy Wang, U.S. Army Research Laboratory, USA

11:45-12:10 Adaptively Compressed Exchange Operator

Lin Lin, University of California, Berkeley and Lawrence Berkeley National Laboratory, USA

Monday, May 9

MS38

Complex Analysis, Optimization, and Herglotz Functions in Passive Electromagnetics and Composite Media - P art IV of IV

10:15 AM-11:45 AM

Room:Society Hill Ballroom A1

For Part 3 see MS27

The aim of this minisymposium is to bring together a diverse group of researchers from mathematics, engineering, and physics that, although working on seemingly distinct topics, use similar tools from complex analysis or optimization theory in which Herglotz or Stieltjes functions are important. This minisymposium will help bring new insights and advancements in the theory of Herglotz functions and its applications by highlighting progress and challenges in the areas of multivariate complex analysis, electromagnetics, and the theory of composites. Topics include Herglotz functions, passive systems, complex analysis, optimization theory, dispersion relations, sum rules, bounds, and applications in electromagnetics and composites.

Organizer: Maxence Cassier University of Utah, USA

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

Organizer: Mihai Putinar University of California, Santa Barbara, USA and Newcastle University, United Kingdom

Organizer: Aaron Welters Florida Institute of Technology, USA

10:15-10:40 Markov Regularization of Multivariate Moment Sequences of Singular Measures

Mihai Putinar, University of California, Santa Barbara, USA and Newcastle University, United Kingdom

10:45-11:10 Fundamental Limits to Wave Scattering in Lossy Media

Owen D. Miller, Massachusetts Institute of Technology, USA

11:15-11:40 Applications of Herglotz Functions in Poroelastic and Elastic Composite Materials

Yvonne Ou, University of Delaware, USA

Monday, May 9

MS39 Numerical Methods in Multiscale Materials

Modelling - Part I of III 10:15 AM-12:15 PM

Room:Society Hill Ballroom A2

For Part 2 see MS50

Multiscale methods are of central importance in the efficient simulation of materials, but it is now evident that the development of robust, scalable methods requires coordinated progress in modelling and numerical analysis. The aim of this minisymposium is to bring together researchers working with knowledge of computational statistical mechanics, molecular dynamics, and stochastic numerics to explore state-ofthe-art development in the methodology of multiscale materials modelling, in order to foster closer contact and facilitate the exchange of ideas and expertise across the different areas.

Organizer: Vagelis Harmandaris University of Crete, Greece

Organizer: Benedict Leimkuhler University of Edinburgh, United Kingdom

Organizer: Xiaocheng Shang University of Edinburgh, United Kingdom

10:15-10:40 Modeling the Mechanics of 2D Layered Heterostructures

Ellad B. Tadmor, University of Minnesota, USA

10:45-11:10 From Atomistic to Systematic Coarse-Grained Models for Molecular Systems

Vagelis Harmandaris, University of Crete, Greece; Evangelia Kalligiannaki, University of Southern California, USA; Markos A. Katsoulakis, University of Massachusetts, Amherst, USA; Petr Plechac, University of Delaware, USA

11:15-11:40 Surface Hopping Algorithms for Mixed Quantum-Classical Dynamics

Jianfeng Lu, Duke University, USA

11:45-12:10 Efficient and Robust Free Energy Calculations in Materials Noam Bernstein, Naval Research Laboratory, USA

Monday, May 9

MS40

Modeling Mechanical Response in Disordered and Structurally Complex Materials Systems - Part IV of IV

10:15 AM-12:15 PM

Room:Cook

For Part 3 see MS29

We propose a minisymposium exploring approaches to the quantification of microstructure with an eye to modeling mechanical response in materials that exhibit disorder and structural complexity. Examples of such systems include glasses, granular media, colloids, and biological systems. Many interesting interconnections can be drawn between these including incompatible embedded metrics that lead to residual stresses, poorly characterized structures that accommodate plasticity and flow, and a need to account for how forces are generated, accommodated and distributed. This minisymposium will bring together materials scientists, physicists, mathematicians and engineers to examine these problems from multiple overlapping perspectives.

Organizer: Michael L. Falk Johns Hopkins University, USA

Organizer: Timothy J. Atherton *Tufts University, USA*

10:15-10:40 Crack Propagation in Bone: The Role of Sacrificial Bonds Ahmed Elbanna, University of Illinois at Urbana-Champaign, USA

10:45-11:10 Motility Driven Glass Transitions in Biological Tissues Lisa Manning, Syracuse University, USA

MS40

Modeling Mechanical Response in Disordered and Structurally Complex Materials Systems -Part IV of IV

10:15 AM-12:15 PM

Room:Cook continued

11:15-11:40 Elastic Free Energy and the Shapes of Growing Tumors

Krishna Garikipati, University of Michigan, USA; Kristen Mills, Rensselaer Polytechnic Institute, USA; Shiva Rudraraju, University of Michigan, USA; Ralf Kemkemer, Universitaet Reutlingen, Germany

11:45-12:10 The Mechanics of Gap Formation in Endothelial Cell Monolayers

Joyjit Chattoraj and Emanuela Del Gado, Georgetown University, USA; C. Corey Hardin, Massachusetts General Hospital, USA; Ramaswamy Krishnan, Beth Israel Deaconess Medical Center, USA

Monday, May 9

MS41

Soft Matter and Complex Biological Systems - Part I of III 10:15 AM-12:15 PM

Room:Flower

For Part 2 see MS52

The purpose of this minisymposium is to bring together active researchers in the field of soft matter materials whose research activities are closely related to various complex biological phenomena, mechanisms and functionality. In recent years, various complex biological systems have been successfully modeled using soft matter models like cell motility, biological gels, ion channel modeling etc.. The SIAM Materials Meeting provides an opportunity for people with diverse background to exchange ideas and forge new collaborations. You are all experts in various related fields involving soft matter modeling, experiments and simulations. It would be ideal to have such a group to discuss current issues and predict future directions in this active interdisciplinary research field.

Organizer: Qi Wang University of South Carolina, USA

Organizer: M. Gregory Forest University of North Carolina at Chapel Hill, USA

Organizer: Jia Zhao University of South Carolina, USA

10:15-10:40 Biological Plywoods

Alejandro D. Rey, McGill University, Canada

10:45-11:10 Modeling Dynamics of Mucous Flows

M. Gregory Forest, University of North Carolina at Chapel Hill, USA; Paula A. Vasquez, University of South Carolina, USA

11:15-11:40 Transport of Charged Particles in Biological Environments.

Chun Liu, Pennsylvania State University, USA

11:45-12:10 Stochastic and Multi-Scale Dynamics of Stem Cells and Developmental Patterning.

Qin Nie, University of California, Irvine, USA

Monday, May 9

MS42

Microscopic Processes and Non-Equilibrium Phenomena in Epitaxial Growth -Part I of III

10:15 AM-11:45 AM

Room:Bromley

For Part 2 see MS53

Epitaxial growth is a process where material is deposited on top of another one and takes on the crystalline orientation of the substrate. It is of technological importance for a variety of applications including the fabrication of opto-electronic devices, catalysis and food processing. The study of microscopic processes of epitaxy pose mathematical challenges. The purpose of this minisymposium is to bring together experts workingon models and computational tools for a fundamental understanding of non-equilibrium processes in epitaxy. These models and methods are deterministic or stochastic and span several length and time scales. from the atomistic to the continuum.

Organizer: Frederic G. Gibou University of California, Santa Barbara, USA

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

Organizer: Christian Ratsch University of California, Los Angeles, USA

10:15-10:40 Island Dynamics Model for Mound Formation: Effect of a Step-Edge Barrier

Christian Ratsch, University of California, Los Angeles, USA

10:45-11:10 Coarse-Graining from Atomistic to Continuum Models for Island and Step Dynamics during Epitaxial Growth and Relaxation James Evans, Ames Laboratory USDOE,

USA

11:15-11:40 Epitaxial Growth of Graphene

Axel Voigt, Technische Universität Dresden, Germany

MS43

Upscaling Models of Crystalline Structures: Analysis and Simulation - Part I of III

10:15 AM-12:15 PM

Room:Claypoole

For Part 2 see MS54

In the recent years, there has been an extensive development of new upscaling schemes for the passage from atomistic to continuum models of crystalline structures. These upscaling schemes incorporate various models such as KMC, discrete Burton-Cabrera- Frank, DFT and continuum PDEs, in statical and dynamical settings. All of these models have their strengths and limitations, and reconciling them as well as highlighting their differences is very important both from a theoretical point of view, and for our understanding of the structure and evolution of crystalline materials in general.

Organizer: Hala A.H. Shehadeh James Madison University, USA

Organizer: Malena I. Espanol University of Akron, USA

10:15-10:40 On the Connection Between Kinetic Monte Carlo and Burton-Cabrera-Frank Theory of Step-Flow in 1+1 Dimensions

Paul Patrone, National Institute of Standards and Technology, USA

10:45-11:10 Hydrodynamic Limit of a KMC Model for a Layered Cake Structure and Facet Formation

Hala A.H. Shehadeh, James Madison University, USA

11:15-11:40 Modeling Effect of Flow on Crystallization Kinetics: From Kinetic Theory to Hydrodynamics

Arvind Baskaran, National Institute of Standards and Technology, USA; Aparna Baskaran, Brandeis University, USA; John Lowengrub, University of California, Irvine, USA

11:45-12:10 Peridynamic Models for Upscaling Crystalline Structures

Pablo Seleson, Oak Ridge National Laboratory, USA

Monday, May 9

MS44

Recent Trends in Micromagnetic Modeling and Analysis - Part I of III

10:15 AM-12:15 PM

Room:Frampton

For Part 2 see MS55

Magnetic materials underlie present and future technologies for information storage. The last two decades have brought major technological breakthroughs in the design of novel magnetic materials and the development of new application concepts for these materials. Simultaneously, recent efforts in micromagnetic modeling and analysis have yielded a deeper understanding of many phenomena observed in magnetic materials. Yet, progress in the material design and use poses further challenges to the mathematical community. The proposed minisymposium brings together scientists working on modeling, analysis, simulation and experimental characterization of the current and emerging magnetic materials and aims to set new directions and define major open problems.

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

Organizer: Valery Slastikov University of Bristol, United Kingdom

10:15-10:40 Current Induced Torques in Magnetic Thin Films and Devices: Physics and Modeling

Andrew Kent, New York University, USA

10:45-11:10 A Mean-Field Model for Spin Dynamics in Multilayered Ferromagnetic Media

Jingrun Chen, *Carlos Garcia-Cervera*, and Xu Yang, University of California, Santa Barbara, USA

11:15-11:40 Magnetic Domains in Thin Ferromagnetic Films with Strong Perpendicular Anisotropy

Hans Knuepfer, University of Heidelberg, Germany; Cyrill B. Muratov, New Jersey Institute of Technology, USA; *Florian Nolte*, Heidelberg University, Germany

11:45-12:10 Homogenization of Composite Ferromagnetic Materials Francois Alouges, University of Paris-Sud, France; *Giovanni Di Fratta*, Ecole Polytechnique, France

Lunch Break

12:15 PM-1:30 PM

Attendees on their own

Poster Spotlights

1:30 PM-2:15 PM Room:Society Hill Ballroom B,C,D,E

Intermission

2:15 PM-2:30 PM

continued in next column

MS45 Metamaterials and Their Recent Applications - Part I of V

2:30 PM-4:30 PM

Room:Society Hill Ballroom B

For Part 2 see MS56

Metamaterials are materials engineered to have properties that have not yet been found in nature. This minisymposium is devoted to recent progress on understanding properties of these materials and their applications. In this minisymposium, the speakers will discuss various types of metamaterials for instance negative index materials, hyperbolic metamaterials, and seismic metamaterials and their applications such as superlensing, cloaking, cloaking via anomalous localized resonance. Different aspects of these materials such as resonance, localized resonance, stability, outgoing conditions, limiting amplitude principle are presented. Both theoretical and numerical aspects are covered.

Organizer: Hoai-Minh Nguyen École Polytechnique Fédérale de Lausanne, Switzerland

2:30-2:55 Superlensing Using Hyperbolic Metamaterials

Eric Bonnetier, Université Grenoble Alpes, France; Hoai-Minh Nguyen, École Polytechnique Fédérale de Lausanne, Switzerland

3:00-3:25 ALR with Maxwell's Equations

Petri Ola and Matti Lassas, University of Helsinki, Finland

3:30-3:55 A Three-Sphere Inequality and Cloaking Using Complementary Media in the Finite Frequency Regime *Loc Nguyen*, University of North

Carolina, Charlotte, USA

4:00-4:25 Uniform Refraction in Negative Refractive Index Materials *Eric Stachura* and Cristian Gutierrez,

Temple University, USA

Monday, May 9

MS46

Analysis. Modeling, and Simulation in Materials Science, in Memory of Peter Smereka - Part I of III

2:30 PM-4:00 PM

Room:Society Hill Ballroom C

For Part 2 see MS57

We were all saddened to learn of Peter's sudden death on Sept. 15. Peter, who was serving as the co-chair of this meeting at the time of his passing, was a great asset to the math-materials community. One of his most memorable traits was his level of participation at conferences. Very few people pay so much attention to what others are presenting. It was rare for him to sit through an entire talk without asking an insightful question; more often several. When Peter helped organize meetings, he encouraged this type of interaction between the audience and the speaker.

Organizer: Tim Schulze University of Tennessee, USA

2:30-2:55 Nonlinear Quantum Mechanics

Bjorn Birnir, University of California, Santa Barbara, USA

3:00-3:25 Modeling Rare Events *Weinan E*, Princeton University, USA

3:30-3:55 Euler Sprays and Optimal Transportation

Robert Pego, Carnegie Mellon University, USA; Jian-Guo Liu, Duke University, USA; Dejan Slepcev, Carnegie Mellon University, USA

Monday, May 9

MS47

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part V of VI

2:30 PM-4:00 PM

Room:Society Hill Ballroom D

For Part 4 see MS36 For Part 6 see MS58

Polycrystalline grain microstructures are ubiquitous among technologically important materials, such as most metals and ceramics. The control of microstructures through processing is crucial to improvement of material properties, such as strength, toughness and electrical conductivity. This minisymposium will focus on understanding and prediction of thermodynamics and kinetics of grain microstructures. The minisymposium will bring together experts from materials science and mathematics and will include talks that range from experiments and modeling to algorithm development and analysis.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Selim Esedoglu University of Michigan, USA

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Dana Zoellner Otto-von-Guericke University, Magdenburg, Germany

2:30-2:55 Phase Field Models of Creep in Polycrystals

James Warren and Arvind Baskaran, National Institute of Standards and Technology, USA

3:00-3:25 Dynamics of Polycrystalline Networks

Martin E. Glicksman, Florida Institute of Technology, USA; Paulo Rios, Centro Universitário FEI, Brazil

3:30-3:55 Thin Film Deposition Using Rarefied Gas Jet

Dr. Sahadev Pradhan, Indian Institute of Science, Bangalore, India
MS48

Mathematics and Algorithms for Excited States of Materials -Part I of II

2:30 PM-4:00 PM

Room:Society Hill Ballroom E

For Part 2 see MS59

Quantitative predictions for excited state phenomena are at the leading edge of modern theories for the electronic structure of materials. These predicative capabilities have a wide range of applications in the design and simulation of new materials for photovoltaics, energy storage and other nanoelectronic devices. In this minisymposium, we bring researchers from both materials science and mathematics to discuss methodologies and algorithms for modeling, computing and analyzing excited state properties of materials. The topics to be covered include but are not limited to many-body perturbation theory and Green's function methods, timedependent density functional theory.

Organizer: Chao Yang Lawrence Berkeley National Laboratory, USA

Organizer: Eric Cances Ecole des Ponts and Inria, France

2:30-2:55 Ab-initio Dynamics from Electronic to Molecular Scales Efthimios Kaxiras, Harvard University, USA

3:00-3:25 Correlated Methods for Periodic Systems Based on Localized Resolution of Identity Technique

Xinguo Ren, University of Science and Technology of China, China

3:30-3:55 Multiscale Modeling and Computation of Optically Manipulated Nano Devices

Di Liu, Michigan State University, USA

Monday, May 9

MS49

Active Polar Gels -Part I of II

2:30 PM-4:30 PM

Room:Society Hill Ballroom A1

For Part 2 see MS60

The hydrodynamic equations of active polar gels model the continuum, macroscopic mechanics of a collection of uniaxial active agents, embedded in a viscous bulk medium, in which internal stresses are induced due to dissipation of energy. The energy-consuming uniaxial polar agents are modeled by a polarization field, which is governed by an equation of motion. The relationship between the strain rate and the stress in the fluid is provided by a constitutive equation. These equations, along with conservation of momentum, provide a continuum hydrodynamic description modeling active polar viscous gels as an energy consuming, anisotropic, non-Newtonian fluid. Within this minisymposium we will discuss modeling aspects, various applications and numerical issues.

Organizer: Axel Voig† Technische Universität Dresden, Germany

2:30-2:55 Collisions of Deformable Cells Lead to Collective Migration

Igor S. Aronson, Argonne National Laboratory, USA

3:00-3:25 Collective Motion of Cells under the Influence of Hydrodynamics

Axel Voigt, Technische Universität Dresden, Germany

3:30-3:55 Modelling the Cell Cytoskeleton as an Active Polar Gel: Cell Deformation and Movement

Rhoda Hawkins, University of Sheffield, United Kingdom

4:00-4:25 Collective Dynamics on Large Scales - A Phase Field Crystal Like Approach

Francesco Alaimo, Technische Universität Dresden, Germany

Monday, May 9 MS50

Numerical Methods in Multiscale Materials Modelling - Part II of III

2:30 PM-4:30 PM

Room:Society Hill Ballroom A2

For Part 1 see MS39 For Part 3 see MS61

Multiscale methods are of central importance in the efficient simulation of materials, but it is now evident that the development of robust, scalable methods requires coordinated progress in modelling and numerical analysis. The aim of this minisymposium is to bring together researchers working with knowledge of computational statistical mechanics, molecular dynamics, and stochastic numerics to explore state-ofthe-art development in the methodology of multiscale materials modelling. in order to foster closer contact and facilitate the exchange of ideas and expertise across the different areas.

Organizer: Vagelis Harmandaris University of Crete, Greece

Organizer: Benedict Leimkuhler University of Edinburgh, United Kingdom

Organizer: Xiaocheng Shang University of Edinburgh, United Kingdom

2:30-2:55 Error Estimates for Transport Coefficients in Molecular Dynamics *Gabriel Stoltz*, Ecole Nationale des Ponts et Chaussées, France

3:00-3:25 Overcoming Bad Scaling Using Ensemble Samplers

Charles Matthews, University of Chicago, USA; Ben Leimkuhler, University of Edinburgh, United Kingdom; Jonathan Weare, University of Chicago, USA

37

MS50

Numerical Methods in Multiscale Materials Modelling - Part II of III

2:30 PM-4:30 PM Room:Society Hill Ballroom A2 continued

3:30-3:55 Accelerated Sampling of Exit Rates for Molecular Dynamics Using a Homotopy Approach

Marcus Weber and *Jannes Quer*, Zuse Institute Berlin, Germany

4:00-4:25 Optimal Control of Multiscale Systems Using Reduced-Order Models

Wei Zhang, Carsten Hartmann, and Juan Cristobal Latorre, Free University of Berlin, Germany; Grigorios Pavliotis, Imperial College London, United Kingdom

Monday, May 9

MS51

Mathematical and Computational Aspects of Nonlocal Models in Materials Science - Part I of V

2:30 PM-4:30 PM

Room:Cook

For Part 2 see MS62

The minisymposium is focused on the recent developments of nonlocal mathematical models arising in peridynamics, dynamics of complex fluid and porous media. These nonlocal models aim to quantitatively and consistently incorporate the effect of subscale phenomena such as discrete particles, cracks, polymeric molecules and microstructure into the continuum model. The talks will address both the analytical and numerical aspects of these models and their implication in our understanding of the behaviors of these materials.

Organizer: Miao-Jung Y. Ou University of Delaware, USA

Organizer: Silvia Jimenez Bolanos *Colgate University, USA*

Organizer: Bacim Alali Kansas State University, USA

2:30-2:55 Propagation of Complex Fracture Using Nonlocal Cohesive Forces

Robert P. Lipton, Louisiana State University, USA

3:00-3:25 On the Consistency Between Nearest-Neighbor Peridynamics and Finite Difference Classical Elasticity

Pablo Seleson, Oak Ridge National Laboratory, USA; Qiang Du, Columbia University, USA; Michael L. Parks, Sandia National Laboratories, USA

3:30-3:55 On the Variational Convergence of a Class of Nonlocal Functionals Related to Peridynamics *Tadele Mengesha*, University of

Tennessee, USA

4:00-4:25 Numerical Approximations for Two-Dimensional Nonlocal Phase-Field Crystal Models by Fourier Spectral Methods

Jiang Yang and Qiang Du, Columbia University, USA

Monday, May 9

MS52

Soft Matter and Complex Biological Systems - Part II of III

2:30 PM-4:30 PM

Room:Flower

For Part 1 see MS41 For Part 3 see MS63

The purpose of this minisymposium is to bring together active researchers in the field of soft matter materials whose research activities are closely related to various complex biological phenomena, mechanisms and functionality. In recent years, various complex biological systems have been successfully modeled using soft matter models like cell motility, biological gels, ion channel modeling etc.. The SIAM Materials Meeting provides an opportunity for people with diverse background to exchange ideas and forge new collaborations. You are all experts in various related fields involving soft matter modeling, experiments and simulations. It would be ideal to have such a group to discuss current issues and predict future directions in this active interdisciplinary research field.

Organizer: Qi Wang University of South Carolina, USA

Organizer: M. Gregory Forest University of North Carolina at Chapel Hill, USA

Organizer: Jia Zhao University of South Carolina, USA

2:30-2:55 Computational Model of Substrate-Based Cell Motility

Igor S. Aronson, Argonne National Laboratory, USA

3:00-3:25 Nonlinearities and Symmetry Breaking in Active Biological Matter *Tanniemola liverpool*, University of Bristol, United Kingdom

38

3:30-3:55 Active Liquid Crystal Models and Applications to Complex Biological Systems

Qi Wang, University of South Carolina, USA and Beijing Computational Science Research Center, China; Jia Zhao, University of South Carolina, USA; Xiaogang Yang, Beijing Computational Science Research Center, China

4:00-4:25 A Multiphasic Complex Fluids Model for Cytokinesis of Eukaryotes

Jia Zhao, University of South Carolina, USA

Monday, May 9

MS53

Microscopic Processes and Non-Equilibrium Phenomena in Epitaxial Growth - Part II of III

2:30 PM-4:00 PM

Room:Bromley

For Part 1 see MS42 For Part 3 see MS64

Epitaxial growth is a process where material is deposited on top of another one and takes on the crystalline orientation of the substrate. It is of technological importance for a variety of applications including the fabrication of opto-electronic devices, catalysis and food processing. The modeling and simulation of epitaxy pose mathematical challenges. The purpose of this minisymposium is to bring together experts working on models and computational tools for a fundamental understanding of non-equilibrium processes in epitaxy. These models and methods are deterministic or stochastic and span several length and time scales, from the atomistic to the continuum.

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

Organizer: Frederic G. Gibou University of California, Santa Barbara, USA

Organizer: Christian Ratsch University of California, Los Angeles, USA

2:30-2:55 Parallel Octree-Based Discretizations for Diffusion Dominated Free Boundary Problems

Frederic G. Gibou, University of California, Santa Barbara, USA

3:00-3:25 Wetting and Dewetting Dynamics of Thin Solid Films

Oliver Pierre-Louis, Université Claude Bernard Lyon 1, France

3:30-3:55 Kinetic Models for Crystalline Misorientations During Coarsening in 2D Materials

Maria Emelianenko, George Mason University, USA

Monday, May 9

MS54

Upscaling Models of Crystalline Structures: Analysis and Simulation -Part II of III

2:30 PM-4:00 PM

Room:Claypoole

For Part 1 see MS43 For Part 3 see MS65

In the recent years, there has been an extensive development of new upscaling schemes for the passage from atomistic to continuum models of crystalline structures. These upscaling schemes incorporate various models such as KMC, discrete Burton-Cabrera-Frank, DFT and continuum PDEs, in statical and dynamical settings. All of these models have their strengths and limitations, and reconciling them as well as highlighting their differences is very important both from a theoretical point of view, and for our understanding of the structure and evolution of crystalline materials in general.

Organizer: Hala A.H. Shehadeh James Madison University, USA

Organizer: Malena I. Espanol University of Akron, USA

2:30-2:55 An Upscaling Procedure for Passing from an Atomistic to a Continuum Model of Multi-Walled Carbon Nanotubes

Malena I. Espanol, Dmitry Golovaty, and J. Patrick Wilber, University of Akron, USA

3:00-3:25 Crystallization for a Brenner-Like Potential

Brittan A. Farmer, University of Minnesota, USA; Selim Esedoglu and Peter Smereka, University of Michigan, USA

3:30-3:55 A Framework to Compute Elastic Deformation Fields from Atomistics: the Key to Automated Identification of Dislocations, Grain Boundaries, and Stacking Faults

Alexander Stukowski, Technische Universität Darmstadt, Germany

LR

Monday, May 9

MS55

Recent Trends in Micromagnetic Modeling and Analysis - Part II of III

2:30 PM-4:30 PM

Room:Frampton

For Part 1 see MS44 For Part 3 see MS66

Magnetic materials underlie present and future technologies for information storage. The last two decades have brought major technological breakthroughs in the design of novel magnetic materials and the development of new application concepts for these materials. Simultaneously, recent efforts in micromagnetic modeling and analysis have yielded a deeper understanding of many phenomena observed in magnetic materials. Yet, progress in the material design and use poses further challenges to the mathematical community. The proposed minisymposium brings together scientists working on modeling, analysis, simulation and experimental characterization of the current and emerging magnetic materials and aims to set new directions and define major open problems.

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

Organizer: Valery Slastikov University of Bristol, United Kingdom

2:30-2:55 Spin Orbit Torques and Chiral Spin Textures in Ultrathin Magnetic Films

Geoffrey Beach, Massachusetts Institute of Technology, USA

3:00-3:25 Dynamical and Static Stabilization Mechanisms for Skyrmions *Benjamin Braun*, University of Kentucky,

USA

3:30-3:55 Ferromagnetic and Antiferromagnetic Skyrmions Oleg Tretiakov, Tohoku University, Japan

4:00-4:25 Current-Induced Dynamics of Chiral Skyrmions

Christof Melcher, RTWH Aachen, Germany Monday, May 9

Coffee Break 4:30 PM-5:00 PM Room:Hamilton Room



MS56

Metamaterials and Their Recent Applications -Part II of V

5:00 PM-6:30 PM

Room:Society Hill Ballroom B

For Part 1 see MS45 For Part 3 see MS67

Metamaterials are materials engineered to have properties that have not yet been found in nature. This minisymposium is devoted to recent progress on understanding properties of these materials and their applications. In this minisymposium, the speakers will discuss various types of metamaterials for instance negative index materials, hyperbolic metamaterials, and seismic metamaterials and their applications such as superlensing, cloaking, cloaking via anomalous localized resonance. Different aspects of these materials such as resonance, localized resonance, stability, outgoing conditions, limiting amplitude principle are presented. Both theoretical and numerical aspects are covered.

Organizer: Hoai-Minh Nguyen École Polytechnique Fédérale de Lausanne, Switzerland

5:00-5:25 On the Black-Hole Phenomenon at Corners of Metamaterials

Anne Sophie Bonnet-Ben Dhia, ENSTA ParisTech, France

5:30-5:55 Plasmonic Coupling Between Two Nanoparticles

Pierre Millien, École Polytechnique Fédérale de Lausanne, Switzerland

6:00-6:25 Spectral Properties of the Neumann-Poincaré Operator and Cloaking by Anomalous Localized Resonance for the Elasto-Static System

Hyeonbae Kang, Inha University, Korea; Kazunori Ando, Ehime University, Japan; Yongkwan Ji and Kyoungsun Kim, Inha University, Korea; Sanghyeon Yu, ETH Zürich, Switzerland

Monday, May 9

MS57

Analysis. Modeling, and Simulation in Materials Science, in Memory of Peter Smereka - Part II of III

5:00 PM-7:00 PM

Room:Society Hill Ballroom C

For Part 1 see MS46 For Part 3 see MS68

We were all saddened to learn of Peter's sudden death on Sept. 15. Peter, who was serving as the co-chair of this meeting at the time of his passing, was a great asset to the math-materials community. One of his most memorable traits was his level of participation at conferences. Very few people pay so much attention to what others are presenting. It was rare for him to sit through an entire talk without asking an insightful question; more often several. When Peter helped organize meetings, he encouraged this type of interaction between the audience and the speaker.

Organizer: Tim Schulze University of Tennessee, USA

5:00-5:25 Kinetic Monte Carlo---A Look Back and a Glance Forward *Tim Schulze*, University of Tennessee, USA

5:30-5:55 A Levelset Method for Modeling the Formation and Self-Organization of Quantum Dots During Epitaxial Growth

Christian Ratsch, University of California, Los Angeles, USA

6:00-6:25 Formulations Treating Stochastic Effects in Thin Film Growth and Relaxation Including Contributions by Peter Smereka

James Evans, Ames Laboratory USDOE, USA

6:30-6:55 Phase Field Models Capturing Surface Diffusion

Axel Voigt, Technische Universität Dresden, Germany

MS58

Recent Developments in Mathematical Modeling of Recrystallization, Grain Growth and Related Phenomena - Part VI of VI

5:00 PM-6:30 PM

Room:Society Hill Ballroom D

For Part 5 see MS47

Polycrystalline grain microstructures are ubiquitous among technologically important materials, such as most metals and ceramics. The control of microstructures through processing is crucial to improvement of material properties, such as strength, toughness and electrical conductivity. This minisymposium will focus on understanding and prediction of thermodynamics and kinetics of grain microstructures. The minisymposium will bring together experts from materials science and mathematics and will include talks that range from experiments and modeling to algorithm development and analysis.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Selim Esedoglu University of Michigan, USA

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Dana Zoellner Otto-von-Guericke University, Magdenburg, Germany

5:00-5:25 Twin Boundary Junction Effects in Grain Growth

David J. Srolovitz and Spencer Thomas, University of Pennsylvania, USA

5:30-5:55 Multi-scale Atomistic Simulations Scheme for Grain Boundaries

Liam Huber, Blazej Grabowski, and Joerg Neugebauer, Max-Planck-Institute for Iron Research, Germany; Joerg Rottler and *Matthias Militzer*, University of British Columbia, Canada

6:00-6:25 Review of Abnormal Grain Growth, New and Old Mechanisms Anthony Rollett, Carnegie Mellon

University, USA

Monday, May 9

MS59

Mathematics and Algorithms for Excited States of Materials -Part II of II

5:00 PM-6:30 PM

Room:Society Hill Ballroom E

For Part 1 see MS48

Quantitative predictions for excited state phenomena are at the leading edge of modern theories for the electronic structure of materials. These predicative capabilities have a wide range of applications in the design and simulation of new materials for photovoltaics, energy storage and other nanoelectronic devices. In this minisymposium, we bring researchers from both materials science and mathematics to discuss methodologies and algorithms for modeling, computing and analyzing excited state properties of materials. The topics to be covered include but are not limited to manybody perturbation theory and Green's function methods, time-dependent density functional theory.

Organizer: Chao Yang Lawrence Berkeley National Laboratory, USA

Organizer: Eric Cances Ecole des Ponts and Inria, France

5:00-5:25 A Mathematical Analysis of the GW Method for Computing Electronic Excited Energies *Gabriel Stoltz*, École des Ponts

ParisTech, France

5:30-5:55 Ab Initio Parametrization of Bond-polarizability Model for Raman Spectroscopy of a-Si:H

David A. Strubbe and Jeffrey C. Grossman, Massachusetts Institute of Technology, USA

6:00-6:25 A New Algorithm for Real-time Time Dependent Density Funcitonal Theory Calculations

Lin-Wang Wang, Lawrence Berkeley National Laboratory, USA

Monday, May 9

MS60 Active Polar Gels -Part II of II

5:00 PM-6:30 PM

Room:Society Hill Ballroom A1

For Part 1 see MS49

The hydrodynamic equations of active polar gels model the continuum, macroscopic mechanics of a collection of uniaxial active agents, embedded in a viscous bulk medium, in which internal stresses are induced due to dissipation of energy. The energyconsuming uniaxial polar agents are modeled by a polarization field, which is governed by an equation of motion. The relationship between the strain rate and the stress in the fluid is provided by a constitutive equation. These equations, along with conservation of momentum, provide a continuum hydrodynamic description modeling active polar viscous gels as an energy consuming, anisotropic, non-Newtonian fluid. Within this minisymposium we will discuss modeling aspects, various applications and numerical issues.

Organizer: Axel Voig† Technische Universität Dresden, Germany

5:00-5:25 Geometry and Topology of Turbulence in Active Nematics

Luca Giomi, Universiteit Leiden, Netherlands

5:30-5:55 A Hybrid Particle-Mesh Method for Incompressible Active Polar Viscous Gels

Ivo F. Sbalzarini, Technische Universität Dresden, Germany

6:00-6:25 Nonlinear Spatiotemporal Dynamics of Active Fluids and Applications to Cell Biomechanics

Rajesh Ramaswamy, Max Planck Institute for Physics of Complex Systems, Germany

MS61 Numerical Methods in Multiscale Materials Modelling - Part III of III

5:00 PM-7:00 PM

Room:Society Hill Ballroom A2

For Part 2 see MS50

Multiscale methods are of central importance in the efficient simulation of materials, but it is now evident that the development of robust, scalable methods requires coordinated progress in modelling and numerical analysis. The aim of this minisymposium is to bring together researchers working with knowledge of computational statistical mechanics, molecular dynamics, and stochastic numerics to explore state-ofthe-art development in the methodology of multiscale materials modelling, in order to foster closer contact and facilitate the exchange of ideas and expertise across the different areas.

Organizer: Vagelis Harmandaris University of Crete, Greece

Organizer: Benedict Leimkuhler University of Edinburgh, United Kingdom

Organizer: Xiaocheng Shang University of Edinburgh, United Kingdom

5:00-5:25 Increasing the Timestep in Molecular Dynamics Simulation

Ben Leimkuhler, University of Edinburgh, United Kingdom

5:30-5:55 Error Analysis of Modified Langevin Dynamics

Zofia Trstanova, Inria Grenoble, France; Gabriel Stoltz, Ecole Nationale des Ponts et Chaussées, France; Stephane Redon, Inria, France

6:00-6:25 Coarse-Graining Strategies for Polymer Systems

Dimitrios Tsagkarogiannis, University of Sussex, United Kingdom; Anastasios Tsourtis and Vagelis Harmandaris, University of Crete, Greece

6:30-6:55 On the Numerical Treatment of Dissipative Particle Dynamics and Related Systems: An Adaptive Formulation

Xiaocheng Shang and Benedict Leimkuhler, University of Edinburgh, United Kingdom Monday, May 9

MS62

Mathematical and Computational Aspects of Nonlocal Models in Materials Science - Part II of V

5:00 PM-6:30 PM

Room:Cook

For Part 1 see MS51 For Part 3 see MS73

The minisymposium is focused on the recent developments of nonlocal mathematical models arising in peridynamics, dynamics of complex fluid and porous media. These nonlocal models aim to quantitatively and consistently incorporate the effect of subscale phenomena such as discrete particles, cracks, polymeric molecules and microstructure into the continuum model. The talks will address both the analytical and numerical aspects of these models and their implication in our understanding of the behaviors of these materials.

Organizer: Miao-Jung Y. Ou University of Delaware, USA

Organizer: Silvia Jimenez Bolanos

Colgate University, USA

Organizer: Bacim Alali Kansas State University, USA

5:00-5:25 Multiscale Structure of Optimally Designed Composites with Nonlocal Constitutive Relations

Elena Cherkaev, University of Utah, USA

5:30-5:55 The Rheology of Non-Dilute Dispersions of Highly Deformable Viscoelastic Particles in Newtonian Fluids

Pedro Ponte Castaneda, University of Pennsylvania, USA

6:00-6:25 Infinite-Order Laminates in a Crystal Plasticity Model with Two Slip Systems

Nathan Albin, Kansas State University, USA

Monday, May 9

MS63

Soft Matter and Complex Biological Systems -Part III of III

5:00 PM-6:30 PM

Room:Flower

For Part 2 see MS52

The purpose of this minisymposium is to bring together active researchers in the field of soft matter materials whose research activities are closely related to various complex biological phenomena, mechanisms and functionality. In recent years, various complex biological systems have been successfully modeled using soft matter models like cell motility, biological gels, ion channel modeling etc.. The SIAM Materials Meeting provides an opportunity for people with diverse background to exchange ideas and forge new collaborations. You are all experts in various related fields involving soft matter modeling, experiments and simulations. It would be ideal to have such a group to discuss current issues and predict future directions in this active interdisciplinary research field.

Organizer: Qi Wang University of South Carolina, USA

Organizer: M. Gregory Forest University of North Carolina at Chapel

Hill, USA

Organizer: Jia Zhao University of South Carolina, USA

5:00-5:25 Modeling Dynamics of and Within the Mitotic Spindle

Michael J. Shelley, Courant Institute of Mathematical Sciences, New York University, USA

5:30-5:55 Active Mechanics of Spindle Positioning

Dan Needleman, Harvard University, USA

6:00-6:25 Confined Spherical Polymer Micelle in a Tube Tunnel

Hui Zhang, Beijing Normal University, China

MS64

Microscopic Processes and Non-Equilibrium Phenomena in Epitaxial Growth -Part III of III

5:00 PM-6:00 PM

Room:Bromley

For Part 2 see MS53

Epitaxial growth is a process where material is deposited on top of another one and takes on the crystalline orientation of the substrate. It is of technological importance for a variety of applications including the fabrication of opto-electronic devices, catalysis and food processing. The study of microscopic processes of epitaxy pose mathematical challenges. The purpose of this minisymposium is to bring together experts workingon models and computational tools for a fundamental understanding of non-equilibrium processes in epitaxy. These models and methods are deterministic or stochastic and span several length and time scales, from the atomistic to the continuum.

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

Organizer: Frederic G. Gibou University of California, Santa Barbara, USA

Organizer: Christian Ratsch University of California, Los Angeles, USA

5:00-5:25 From Atomistic Dynamics to Mesoscale Descriptions of Crystal Growth

Dionisios Margetis, University of Maryland, College Park, USA

5:30-5:55 Formation of Moire Patterns in Ultra Thin Heteroepitaxial Films *Ken Elder*, Oakland University, USA Monday, May 9

MS65

Upscaling Models of Crystalline Structures: Analysis and Simulation -Part III of III

5:00 PM-6:30 PM

Room: Claypoole

For Part 2 see MS54

In the recent years, there has been an extensive development of new upscaling schemes for the passage from atomistic to continuum models of crystalline structures. These upscaling schemes incorporate various models such as KMC, discrete Burton-Cabrera-Frank, DFT and continuum PDEs, in statical and dynamical settings. All of these models have their strengths and limitations, and reconciling them as well as highlighting their differences is very important both from a theoretical point of view, and for our understanding of the structure and evolution of crystalline materials in general.

Organizer: Hala A.H. Shehadeh James Madison University, USA

Organizer: Malena I. Espanol University of Akron, USA

5:00-5:25 Coarse-Grained Modeling and Simulations of a Carbon Nanotube Forest Interacting with a Rigid Substrate

J. Patrick Wilber, University of Akron, USA

5:30-5:55 Magnetism Pathways in Transition Metal Substituted Graphene: A DFT study

Costel Constantin, James Madison University, USA

6:00-6:25 A Bending Theory for Nematic Elastomers

Paul Plucinsky and Kaushik Bhattacharya, California Institute of Technology, USA

Monday, May 9

MS66

Recent Trends in Micromagnetic Modeling and Analysis - Part III of III

5:00 PM-7:00 PM

Room:Frampton

For Part 2 see MS55

Magnetic materials underlie present and future technologies for information storage. The last two decades have brought major technological breakthroughs in the design of novel magnetic materials and the development of new application concepts for these materials. Simultaneously, recent efforts in micromagnetic modeling and analysis have yielded a deeper understanding of many phenomena observed in magnetic materials. Yet, progress in the material design and use poses further challenges to the mathematical community. The proposed minisymposium brings together scientists working on modeling, analysis, simulation and experimental characterization of the current and emerging magnetic materials and aims to set new directions and define major open problems.

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

Organizer: Valery Slastikov University of Bristol, United Kingdom

5:00-5:25 Dynamics in Strongly Spin-Torque-Driven Magnetic Thin Film Nano-Structures

Jonathan Sun, IBM T.J. Watson Research Center, USA

5:30-5:55 Domain Wall Dynamics in Magnetic Nanostructures

Arseni Goussev, Northumbria University, United Kingdom; Ross Lund, New Jersey Institute of Technology, USA; Jonathan Robbins and Valeriy Slastikov, University of Bristol, United Kingdom; Oleg Tretiakov, Tohoku University, Japan; S Vasylkevych, University of Bristol, United Kingdom

MS66

Recent Trends in Micromagnetic Modeling and Analysis - Part III of III

5:00 PM-7:00 PM

Room:Frampton continued

6:00-6:25 Structure, Stability and Existence of 360 Degree Walls

Antonio Capella Kort, Universidad Nacional Autónoma de México, Mexico; Hans Knuepfer, University of Heidelberg, Germany; Cyrill B. Muratov, New Jersey Institute of Technology, USA

6:30-6:55 Charged Boundary-Layer Domain Walls in Thin Ferromagnetic Films

Ross Lund and Cyrill B. Muratov, New Jersey Institute of Technology, USA; Valeriy Slastikov, University of Bristol, United Kingdom

Dinner Break

7:00 PM-8:00 PM Attendees on their own

Monday, May 9

PP1

Poster Session 8:00 PM-10:00 PM

Room:Hamilton Room

Some Characteristics of Resonant Transmission of a Wave Pulse

Gayan S. Abeynanda and Stephen P. Shipman, Louisiana State University, USA

Modeling Shear Banding in Amorphous Solids Using Shear Transformation Zone Theory

Darius Alix-Williams and Michael L. Falk, Johns Hopkins University, USA

A Non-Affine, Conformation Tensor-Based, Viscoelastic Fluid Model

Antony N. Beris, Paul Mwasame, and Norman Wagner, University of Delaware, USA

Three-Dimensional Simulations of Strain Localization in Metallic Glasses

Nicholas M. Boffi and Chris H. Rycroft, Harvard University, USA

Thermal Fluctuations and Elastic Relaxation in the Compressed Exponential Dynamics of Colloidal Gels

Mehdi Bouzid and Emanuela DelGado, Georgetown University, USA

Effect of Viscosity on Propagation of MHD Waves in Astrophysical Plasma Alemayehu Cherkos, Kotebe University

College, Ethiopia

Fully Optimized Second-Order Estimates for the Macroscopic Response of Porous Viscoplastic Materials

Shuvrangsu Das and Pedro Castañeda, University of Pennsylvania, USA

Defect Structures Around Two Colloidal Particles in a Nematic Liquid Crystal Paula Dassbach, University of

Minnesota, USA

Shape Minimization Problems for Structured Materials

Andrew Debenedictis and Timothy J. Atherton, Tufts University, USA

Homogenization Theory for the Prediction of Obstructed Solute Diffusivity in Macromolecular Solutions

Preston Donovan, University of Maryland, Baltimore County, USA; Yasaman Chehreghanianzabi, Saint Louis University, USA; Muruhan Rathinam, University of Maryland, Baltimore County, USA; Silviya Zustiak, Saint Louis University, USA

Minimizer Describing Configuration of Nematic Liquid Crystal Between Cylinders with a Core Surface Penalty

Ashley Earls and Lindsey Hiltner, University of Minnesota, USA

On Some Stochastic Singular Integro-Partial Differential Equations and the Parabolic Transform

Mahmoud M. El-Borai and Khairia E. El-Nadi, Alexandria University, Egypt

A Mechano-Hydraulic Model of Intracranial Pressure Dynamics

Davis Evans, Corina Drapaca, and Joseph Cusumano, Pennsylvania State University, USA

Phase-Field Modeling of Alloy Solidification Using Quaternions and Calphad Input

Jean-Luc Fattebert, Lawrence Livermore National Laboratory, USA

Nucleation and Growth of Cavities in Gels

Robert Foldes and Maria-Carme Calderer, University of Minnesota, USA

Second-Order Homogenization Estimates for the Yield Domain of Composite Materials

Joshua Furer and Pedro Ponte-Castañeda, University of Pennsylvania, USA

Discontinuous Galerkin Methods For Modeling Reactive Interfaces in Photoelectrochemical Solar Cells

Michael D. Harmon, Institute for Computational Engineering and Sciences, USA

Using Correlation Coefficient for Determining Suitability of Eddy Current Testing for Quality Control of Heat Treated Steel

Javeria Hashmi, National University of Sciences and Technology, Pakistan

Modeling Viral DNA Packing in a 2D Circular Domain

Lindsey Hiltner, University of Minnesota, USA

Deformation in Metallic Glass: Connecting Atoms to Continua

Adam R. Hinkle, Johns Hopkins University, USA

An Autogenous Friction Stir Spot Welding Rig for Modelling Heat Generation in Friction Stir Processing

Patryk Jedrasiak, Harvard University, USA; Hugh Shercliff, University of Cambridge, United Kingdom; Chris H. Rycroft, Harvard University, USA

Hybrid Reduced Basis Method and Generalized Polynomial Chaos for Stochastic Partial Differential Equations

Jiahua Jiang, University of Massachusetts, Dartmouth, USA

Stability of Multiscale/multiphysics Simulation of Laser Propagation in Optically-Active Semiconductors

Brent Kraczek and Jaroslaw Knap, U.S. Army Research Laboratory, USA

VoroTop: Voronoi Cell Topology Visualization and Analysis Toolkit

Emanuel A. Lazar, Jian Han, and David J. Srolovitz, University of Pennsylvania, USA

A Computational Framework for Scale Bridging in Multiscale Simulations

Kenneth Leiter, Jaroslaw Knap, Brian Barnes, Richard Becker, and Oleg Borodin, U.S. Army Research Laboratory, USA

Brittle to Ductile Transition in a Model of Sheared Granular Materials

Xiao Ma and Ahmed Elbanna, University of Illinois at Urbana-Champaign, USA

Direct Structure-Property Relations Mining in Scanning Tunneling Microscopy: Markov Random Field and Convolutional Neural Network Approach

Artem Maksov, University of Tennessee, Knoxville and Oak Ridge National Laboratory, USA; Maxim Ziatdinov, Oak Ridge National Laboratory, USA; Shintaro Fujii and Manabu Kiguchi, Tokyo Institute of Technology, Japan; Shuhei Higashibayashi, Institute for Molecular Science, Japan; Hidehiro Sakurai, Osaka University, Japan; Sergei Kalinin and Bobby Sumpter, Oak Ridge National Laboratory, USA

Flow of a Drilling Fluid Between Two Rotating Cylinders

Mehrdad Massoudi, National Energy Technology Laboratory, USA; Weitao Wu, Carnegie Mellon University, USA

Resonant Electromagnetic Scattering in Layered Media with Random Fabrication Errors

Emily A. Mchenry, Louisiana State University, USA

Parameter Identification for Creep Modeling in Polymers for Accurate Manufacture

Ali Mohammadi, Mads Rostgaard Sonne, Giuseppe Dalla Costa, Daniel Gonzalez-Madruga, Leonardo De Chiffre, and Jesper Henri Hattel, Technical University of Denmark, Denmark

Topology Optimization of Hyperelastic Continua

Trung Pham, Christopher Hoyle, and Yue Zhang, Oregon State University, USA; Tam H. Nguyen, Surbana Jurong Private Limited, Singapore

General Theory of Spontaneous Emission Near Exceptional Points

Adi Pick, Harvard University, USA; Bo Zhen and Owen D. Miller, Massachusetts Institute of Technology, USA; Chia Hsu, Yale University, USA; Felipe Hernandez, Massachusetts Institute of Technology, USA; Alejandro Rodriguez, Princeton University, USA; Marin Soljacic and Steven Johnson, Massachusetts Institute of Technology, USA

Kinetics of the Triple Line in Solid-state Wetting

Olivier Pierre-Louis, CNRS and Universite Claude Bernard, France; Ashwani Tripathi, University Claude Bernard, Lyon, France

Coarse-Graining in Metallic Glasses from Molecular Dynamics to Continua

Dihui Ruan, Adam R. Hinkle, and Michael D. Shields, Johns Hopkins University, USA; Chris H. Rycroft, Harvard University, USA; Michael L. Falk, Johns Hopkins University, USA

Discrete Systems with Degenerated Growth

Mathias Schäffner and Stefan Neukamm, Technische Universität Dresden, Germany; Anja Schlömerkemper, University of Würzburg, Germany

Approximate Global Minimizers to Pairwise Interaction Problems

David Shirokoff, New Jersey Institute of Technology, USA

Homogenized Response of Porous Plastic Single Crystals

Dawei Song and Pedro Ponte Castañeda, University of Pennsylvania, USA

Microscale FEA Homogenization Procedure for Use in Elastography Inversions

Assimina A. Pelegri and *Daniel Sullivan*, Rutgers University, USA

Phase Delay for a *b*-Function Model of Viscoelastic Behaviour

John E. Tibballs, NIOM, Nordic Institute for Dental Materials, Norway

Local Rearrangements of Droplets in a Dense Emulsion Under Shear

Vishwas Venkatesh, Sudeep Dutta, Emanuela Del Gado, and Daniel Blair, Georgetown University, USA

Computing Links Between Effective Tensors of Pairs of Fiber-Reinforced Elastic Composites with the Same Microstructure

Patrick M. Wynne, Hansen Pei, and Abe Lyle, Temple University, USA

Multiscale Material Model Development for Accident Tolerant Fuels: Bottom-Up

Jianguo Yu, Jason Hales, and Yongfeng Zhang, Idaho National Laboratory, USA

PP1 Poster Session

8:00 PM-10:00 PM

Room:Hamilton Room

continued

On the Mathematical Structure of the Laws Governing the Fundamental Forces of Nature: A New Axiomatic Matrix Approach

Ramin Zahedi, Hokkaido University, Japan

Toward a Variantional Principle of Space Charge Stimulated Discharge in Electron Irradiated PMMA

Xuewei Zhang, Texas A&M University, USA

Transformation Groups and Discrete Structures in Continuum Description of Defective Crystals

Maxim Zyskin, University of Nottingham, United Kingdom

Tuesday, May 10

Registration 7:30 AM-5:30 PM Room:Society Hill Ballroom Foyer

Remarks

8:00 AM-8:15 AM Room:Society Hill Ballroom B,C,D,E

IP6 Transforming Molecular Modelling with Applied Mathematics

8:15 AM-9:00 AM

Room:Society Hill Ballroom B,C,D,E

In this talk I will describe our work over the past decade in pushing the boundaries of molecular simulation technology with the help of applied mathematics. Examples include using kernel methods from machine learning to improve sampling efficiency, systematic and controlled coarse graining both from quantum mechanical methods to interatomic potentials and from the latter to united atom models. Even well established ideas such as preconditioning have not fully penetrated the materials modelling field. Most of these topics are linked by the notion of locality of interactions, a comprehensive mathematical treatment of which is still in the making.

Gábor Csányi University of Cambridge, United Kingdom

Tuesday, May 10

IP7 Epitaxial Graphene Growth 9:00 AM-9:45 AM

Room:Society Hill Ballroom B,C,D,E

The epitaxial growth of graphene on copper foils is a complex process, influenced by thermodynamic, kinetic, and growth parameters, often leading to diverse island shapes including dendrites, squares, stars, hexagons, butterflies, and lobes. We introduce a phase-field model that provides a unified description of these diverse growth morphologies and compare the model results with experiments. We develop a minimal microkinetic model in order to relate the deposition rate with the partial pressures, to assess the importance of the different chemical species that might attach to the graphene edge. We also build a model for the kinetic coefficient, in this multiple species context. Our main assumption is that different species attach depending on the decoration of hydrogen on the interface, and hence their respective attachment- detachment coefficients should depend on this decoration. Our model explicitly accounts for the anisotropies in the energies of growing graphene edges, kinetics of attachment of carbon at the edges, and the crystallinity of the underlying copper substrate (through anisotropy in surface diffusion). We show that anisotropic diffusion has a very important, counterintuitive role in the determination of the shape of islands, and we present a "phase diagram" of growth shapes as a function of growth rate for different copper facets. Our results are shown to be in excellent agreement with growth shapes observed for high symmetry facets such as (111) and (001) as well as for high-index surfaces such as (221) and (310).

John Lowengrub University of California, Irvine, USA

Coffee Break 9:45 AM-10:15 AM Room:Hamilton Room



MS67 Metamaterials and Their Recent Applications -Part III of V

10:15 AM-12:15 PM

Room:Society Hill Ballroom B

For Part 2 see MS56 For Part 4 see MS77

Metamaterials are materials engineered to have properties that have not yet been found in nature. This minisymposium is devoted to recent progress on understanding properties of these materials and their applications. In this minisymposium, the speakers will discuss various types of metamaterials for instance negative index materials, hyperbolic metamaterials, and seismic metamaterials and their applications such as superlensing, cloaking, cloaking via anomalous localized resonance. Different aspects of these materials such as resonance, localized resonance, stability, outgoing conditions, limiting amplitude principle are presented. Both theoretical and numerical aspects are covered.

Organizer: Hoai-Minh Nguyen École Polytechnique Fédérale de Lausanne, Switzerland

10:15-10:40 Electromagnetic Waves in 2D Honeycomb Structures

James P. Lee-Thorp and *Michael I. Weinstein*, Columbia University, USA; Yi Zhu, Tsinghua University, China

10:45-11:10 On Scattering Resonances of Subwavelength Metallic Gratings

Faouzi Triki, Universite Joseph Fourier, France; Eric Bonnetier, Université Grenoble Alpes, France; Abdelfettah Gtet, Universite Joseph Fourier, France

11:15-11:40 High Frequency Homogenization for Traveling Waves

Davit Harutyunyan and *Graeme W*. *Milton*, University of Utah, USA; Richard Craster, Imperial College London, United Kingdom

11:45-12:10 Weyl Modes and Periodicity-Changing Mechanisms in Mechanaical Metamaterials

Bryan G. Chen, University of Massachusetts, USA; David Zeb Rocklin, University of Michigan, USA; Martin Falk, Massachusetts Institute of Technology, USA; Vincenzo Vitelli, Universiteit Leiden, The Netherlands; Tom Lubensky, University of Pennsylvania, USA

Tuesday, May 10

MS68

Analysis. Modeling, and Simulation in Materials Science, in Memory of Peter Smereka - Part III of III

10:15 AM-12:15 PM

Room:Society Hill Ballroom C

For Part 2 see MS57

We were all saddened to learn of Peter's sudden death on Sept. 15. Peter, who was serving as the co-chair of this meeting at the time of his passing, was a great asset to the math-materials community. One of his most memorable traits was his level of participation at conferences. Very few people pay so much attention to what others are presenting. It was rare for him to sit through an entire talk without asking an insightful question; more often several. When Peter helped organize meetings, he encouraged this type of interaction between the audience and the speaker.

Organizer: Tim Schulze University of Tennessee, USA

10:15-10:40 Large Scale Simulations for a Simple Recrystallization Model via Diffusion Generated Motion

Selim Esedoglu, University of Michigan, USA; Matt Elsey, Courant Institute of Mathematical Sciences, New York University, USA; Peter Smereka, University of Michigan, USA

10:45-11:10 Examining Two-dimensional Ordering from Isotropic Interactions

Ken Elder, Oakland University, USA; Simiso Mkhonta, University of Swaziland, Swaizland; Zhi-Feng Huang, Wayne State University, USA

11:15-11:40 Sensitivity and Parametrization for Multiscale KMC Simulations

Petr Plechac, University of Delaware, USA

11:45-12:10 Modeling Elastic Energy of Alloys: Potential Pitfalls of Continuum Treatments

Arvind Baskaran, National Institute of Standards and Technology, USA; Christian Ratsch, University of California, Los Angeles, USA; Peter Smereka, University of Michigan, USA

MS69

Efficient Numerical Methods and Analytical Techniques for Defect Problems -Part I of V

10:15 AM-12:15 PM

Room:Society Hill Ballroom D

For Part 2 see MS79

Defects in crystalline materials, such as vacancies, dislocations, cracks, grain boundaries and surfaces, play important roles in the mechanical, electronic, and plastic properties of these materials. The complexity of the microstructures of these defects and their evolution at various length and time scales presents new challenges for numerical simulations and analytical modeling. The speakers in this minisymposium will discuss recent advances in the aspects of efficient numerical methods and analytical techniques as well as the obtained new findings for these defect problems

Organizer: Yang Xiang

Hong Kong University of Science and Technology, Hong Kong

10:15-10:40 A Peierls-Nabarro Model of Semicoherent Interfaces

David J. Srolovitz and Shuyang Dai, University of Pennsylvania, USA; Yang Xiang, Hong Kong University of Science and Technology, Hong Kong

10:45-11:10 A Kinetic Monte Carlo Model for Grain Boundary Motion Driven by Curvature

Tim Schulze and Kyle Golenbiewski, University of Tennessee, USA

11:15-11:40 Study the Formation of Microstructure for Highly Reversible Martensitic Materials

Xian Chen, Hong Kong University of Science and Technology, Hong Kong

11:45-12:10 Atomistic-to-Continuum Coupling for Multilattices Through Blending

Derek Olson, University of Minnesota, USA; Xingjie Li, University of North Carolina, Charlotte, USA; Christoph Ortner, University of Warwick, United Kingdom; Mitchell Luskin, University of Minnesota, USA Tuesday, May 10

MS70

Growth, Instabilities and Evolutions of Thin Films and Micro/Nanostructures -Part I of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom E

For Part 2 see MS80

The focus of the interdisciplinary minisymposium is on continuum and discrete models of growth, patterning and formation of thin solid films and structures, as well as on analytical and numerical methods that drive such models. The speakers will describe their recent research that highlights the combination of experiment and theory, and includes such diverse phenomena as coarsening, de-wetting, directed selforganization, and phase transitions.

Organizer: Mikhail V. Khenner Western Kentucky University, USA

Organizer: Stephen J. Watson University of Glasgow, Scotland, United Kingdom

10:15-10:40 G-Equivariant Theory of Coarsening Beyond the Dynamic Scaling Hypothesis

Stephen J. Watson, University of Glasgow, Scotland, United Kingdom

10:45-11:10 Thin Film De-Wetting in the Presence of Long-Range and Oscillatory Interactions

Leonardo Golubovic, West Virginia University, USA

11:15-11:40 Directed Self-Organization with Long-Range Forces: A Dynamical Approach

Jean-Noel Aqua, Pierre and Marie Curie University, Institut des NanoSciences de Paris, France

11:45-12:10 Phase Transition Fronts in Systems with Subdiffusion

Alexander Nepomnyashchy, Technion Israel Institute of Technology, Israel; Vladimir A. Volpert, Northwestern University, USA

Tuesday, May 10

MS71

Inverse Problems in Materials Science -Part I of IV

10:15 AM-11:45 AM

Room:Society Hill Ballroom A1

For Part 2 see MS81

This minisymposium focuses on inverse problems arising in estimating the constitutive parameters of a material (e.g. its conductivity) from indirect measurements (e.g. the voltage and current on the boundary of the material). Inverse problems have many applications such as nondestructive testing, medical imaging, and climate change. The goal of this minisymposium is to highlight a broad spectrum of research results on applications of inverse problems to material sciences.

Organizer: Andrew E. Thaler Institute for Mathematics and its Applications, USA

Organizer: Fernando Guevara Vasquez

University of Utah, USA

Organizer: Maxence Cassier University of Utah, USA

10:15-10:40 New Methods for Imaging

Graeme W. Milton, University of Utah, USA

10:45-11:10 Increasing Stability for Inverse Problems

Ru-Yu Lai, University of Minnesota, USA

11:15-11:40 Converting Strain Maps into Elasticity Maps for Materials with Small Contrast

Cedric Bellis and Pierre M. Suquet, CNRS, France

MS72

Multiscale Behaviour of Deterministic and Probabilistic Material Models - Part I of III

10:15 AM-11:45 AM

Room:Society Hill Ballroom A2

For Part 2 see MS82

This minisymposium addresses new results in the application of variational multiscale methods to systems related to materials science. We will discuss recent progress on coupling atomistic scales with continuum scales. Our main focus will be the statics and dynamics of defects such as dislocations.

Organizer: Florian Theil University of Warwick, United Kingdom

Organizer: Mark Peletier Technische Universiteit Eindhoven, The Netherlands

10:15-10:40 Connecting Atomistic and Continuum Models of Nonlinear Elasticity

Julian Braun, University of Augsburg, Germany

10:45-11:10 Derivation of Self Interaction Energy for Dislocations

Sergio Conti, University of Bonn, Germany; Adriana Garroni, Universita di Roma "La Sapienza," Italy; Stefan Mueller, University of Bonn, Germany; Michael Ortiz, California Institute of Technology, USA

11:15-11:40 Convergence of Interaction-Driven Evolutions of Dislocations

Lucia Scardia, University of Bath, United Kingdom

Tuesday, May 10

MS73

Mathematical and Computational Aspects of Nonlocal Models in Materials Science -Part III of V

10:15 AM-12:15 PM

Room:Cook

For Part 2 see MS62 For Part 4 see MS83

The minisymposium is focused on the recent developments of nonlocal mathematical models arising in peridynamics, dynamics of complex fluid and porous media. These nonlocal models aim to quantitatively and consistently incorporate the effect of subscale phenomena such as discrete particles, cracks, polymeric molecules and microstructure into the continuum model. The talks will address both the analytical and numerical aspects of these models and their implication in our understanding of the behaviors of these materials.

Organizer: Miao-Jung Y. Ou University of Delaware, USA

Organizer: Silvia Jimenez Bolanos *Colgate University, USA*

Organizer: Bacim Alali Kansas State University, USA

10:15-10:40 Wormlike Micellar Solutions: Nonlocality and Shearbanding

L. Pamela Cook, University of Delaware, USA; Lin Zhou, New York City College of Technology, USA

10:45-11:10 On the Memory Terms in the Wave Equations for Poroelastic Materials

Miao-Jung Y. Ou, University of Delaware, USA

11:15-11:40 Energetic Variational Approaches for General Diffusion of Charged Particles.

Chun Liu, Pennsylvania State University, USA

11:45-12:10 A Nonlocal Diffusion Model with Variable Horizons

Yunzhe Tao and Qiang Du, Columbia University, USA

Tuesday, May 10

MS74

Multiscale Modeling Methods for Complex Fluids and Soft Matter - Part I of III

10:15 AM-12:15 PM

Room:Flower

For Part 2 see MS84

This minisymposium focuses on multiscale methods for modeling complex fluids and soft matter by concurrent coupling of macroscopic descriptions and microscopic or mesoscopic dynamics. It will include talks on theory, algorithms and diverse applications of various multiscale methods, such as, domain decomposition method, heterogeneous multiscale method, multiscale finite element/volume method, adaptive resolution scheme, multi-fidelity information fusion and others. With increasing attention on energy materials, bio-inspired materials and material assembly research, this minisymposium will bring together the researchers working on multiscale modeling to share insights and to discuss progress of key challenges in this field.

Organizer: Xin Bian Brown University, USA

Organizer: Wenxiao Pan Pacific Northwest National Laboratory, USA

10:15-10:40 Hydrodynamic Fluctuations of Particle Dynamics Coupled with Continuum X Bian, Brown University, USA

10:45-11:10 Adaptive Resolution Simulation of Supramolecular Water Models

Matej Praprotnik, National Institute of Chemistry, Slovenia

11:15-11:40 Equation-Free Approach to Modeling Complex/multiscale Systems

Minseok Choi, Princeton University, USA

11:45-12:10 Internal-flow Multiscale Method

Matthew K. Borg, University of Edinburgh, United Kingdom

MS75 Computational Methods for Materials Science - Part I of II

10:15 AM-12:15 PM

Room:Bromley

For Part 2 see MS85

The objective of the minisymposium is to bring together researchers in the field of computational material sciences and to review recent advances in this field. Various topics will be covered in the presentations: numerical methods for ab-initio calculations, resolution of multiscale partial differential equations, umbrella sampling, diffusion molecular dynamics, as well as replica-exchange free energy calculations.

Organizer: David Aristoff Colorado State University, USA

Organizer: Olivier Pinaud Colorado State University, USA

10:15-10:40 Real-Space and Real-Time First-Principle Electronic Structure Calculations Using the FEAST Algorith

Eric Polizzi, University of Massachusetts, Amherst, USA

10:45-11:10 Optimal Numerical Approaches to the Stochastic Homogenization of Elliptic Equations and to the Stochastic Drift-Diffusion-Poisson System

Clemens Heitzinger, Caroline Geiersbach, and Leila Taghizadeh, Vienna University of Technology, Austria

11:15-11:40 Magnetic Field-Induced Pattern Formation in Smectic A Liquid Crystals

Carlos Garcia-Cervera, University of California, Santa Barbara, USA; Sookyung Joo, Old Dominion University, USA; Tiziana Giorgi, New Mexico State University, USA

11:45-12:10 Morphologies of Semi-Flexible Polymers in Confinement

David Ackerman and Baskar Ganapathysubramanian, Iowa State University, USA Tuesday, May 10

MS76 Nonlinear Waves in Lattices -Part I of III

10:15 AM-12:15 PM

Room:Claypoole

For Part 2 see MS86

Many problems in materials science concern phenomena where the interplay between discreteness and nonlinearity of the medium leads to the formation of nonlinear waves. Examples include emergence of localized excitations in metamaterials and defect propagation in crystal lattices. This minisymposium features presentations of recent theoretical and experimental results by leading experts in nonlinear lattice dynamics, with an emphasis on promising mathematical developments and novel applications in materials science. It aims to facilitate a fruitful exchange of ideas among mathematicians, physicists and engineers working in this field and identify future directions and open problems.

Organizer: Anna Vainchtein University of Pittsburgh, USA

Organizer: Yuli Starosvetsky Technion - Israel Institute of Technology, Israel

10:15-10:40 Solitary Waves in a Lattice with Competing Interactions

Anna Vainchtein, University of Pittsburgh, USA; Lev Truskinovsky, Ecole Polytechnique, France

10:45-11:10 Energy Spreading in Strongly Nonlinear Lattices: From Nonlinear Diffusion to Second Sound Arkady Pikovsky, University of Potsdam,

Germany

11:15-11:40 2D Wave Channeling in the Locally Resonant Discrete Structures

Yuli Starosvetsky, Technion - Israel Institute of Technology, Israel

11:45-12:10 Twist-Stretch Phase Boundaries in Bi-Stable Chains

Prashant K. Purohit, University of Pennsylvania, USA

Tuesday, May 10 Lunch Break 12:15 PM-1:30 PM Attendees on their own

SIAG/MS Business Meeting

1:30 PM-2:15 PM

Room:Society Hill Ballroom B,C,D,E

Complementary byerages will be served.



Intermission

2:15 PM-2:30 PM

MS77 Metamaterials and Their Recent Applications -Part IV of V

2:30 PM-4:00 PM

Room:Society Hill Ballroom B

For Part 3 see MS67 For Part 5 see MS87

Metamaterials are materials engineered to have properties that have not yet been found in nature. This minisymposium is devoted to recent progress on understanding properties of these materials and their applications. In this minisymposium, the speakers will discuss various types of metamaterials for instance negative index materials, hyperbolic metamaterials, and seismic metamaterials and their applications such as superlensing, cloaking, cloaking via anomalous localized resonance. Different aspects of these materials such as resonance, localized resonance, stability, outgoing conditions, limiting amplitude principle are presented. Both theoretical and numerical aspects are covered.

Organizer: Hoai-Minh Nguyen École Polytechnique Fédérale de Lausanne, Switzerland

2:30-2:55 Outgoing Wave Conditions in Photonic Crystals and Transmission Properties at Interfaces

Ben Schweizer, Technische Universität Dortmund, Germany

3:00-3:25 Asymptotic Theory and Experiments on Seismic Metamaterials

Sebastien Guenneau, Aix-Marseille Université, France

3:30-3:55 On the Effect of Dissipation on Anomalous Localized Resonance Phenomena with Applications to Cloaking and Superlensing

Daniel Onofrei, University of Houston, USA; Andrew E. Thaler, Institute for Mathematics and its Applications, USA

Tuesday, May 10

MS78

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part I of VII

2:30 PM-4:30 PM

Room:Society Hill Ballroom C

For Part 2 see MS88

Colloidal nematic liquid crystals arise in a host of new applications including electrophoresis, microfluidic and display devices. Chromonic liquid crystals offer new perspectives and modeling tools in biology, e.g., in studies of DNA encapsulation. Both areas add new perspectives and challenges across liquid crystal research, including newly observed defect structures and novel liquid crystal flow problems. This minisymposium will focus on understanding of defects, flows with charged particles, mechanical properties of encapsulated anisotropic systems, as well as other related problems. The minisymposium will bring together physicists, mathematicians, and biologists who will discuss their recent work encompassing experiments, modeling, and analysis

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Maria-Carme Calderer University of Minnesota, USA

Organizer: Oleg Lavrentovich Kent State University, USA

2:30-2:55 The Topology of Defects in Smectics

Randall Kamien, University of Pennsylvania, USA

3:00-3:25 Defects in Smectic C Liquid Crystals

Daniel Phillips and Lidia Mrad, Purdue University, USA

3:30-3:55 Smectic A Liquid Crystals Under Applied Field in 3D

Sookyung Joo, Old Dominion University, USA

4:00-4:25 Colloidal and Chiral Stabilization of Knotted Nematic Braids Slobodan Žumer, University of Ljubljana & Jozef Stefan Institute, Slovenia

Tuesday, May 10

MS79

Efficient Numerical Methods and Analytical Techniques for Defect Problems -Part II of V

2:30 PM-4:30 PM

Room:Society Hill Ballroom D

For Part 1 see MS69 For Part 3 see MS89

Defects in crystalline materials, such as vacancies, dislocations, cracks, grain boundaries and surfaces, play important roles in the mechanical, electronic, and plastic properties of these materials. The complexity of the microstructures of these defects and their evolution at various length and time scales presents new challenges for numerical simulations and analytical modeling. The speakers in this minisymposium will discuss recent advances in the aspects of efficient numerical methods and analytical techniques as well as the obtained new findings for these defect problems.

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

2:30-2:55 A New Proof of Convergence to Motion by Mean Curvature for the Bence-Merriman-Osher Algorithm

Drew Swartz, Booz Allen Hamilton, USA; *Aaron Yip*, Purdue University, USA

3:00-3:25 Variational Models for Crystal Image Analysis

Jianfeng Lu, Duke University, USA; Benedikt Wirth, Universität Münster, Germany; Haizhao Yang, Duke University, USA

3:30-3:55 Energy Scaling and Asymptotic Properties of Step Bunching in Epitaxial Growth with Elasticity Effects

Tao Luo and Yang Xiang, Hong Kong University of Science and Technology, Hong Kong; Aaron Nung Kwan Yip, Purdue University, USA

4:00-4:25 Defect Identification and Analysis Via Topology

Emanuel A. Lazar, Jian Han, and David J. Srolovitz, University of Pennsylvania, USA

MS80

Growth, Instabilities and Evolutions of Thin Films and Micro/Nanostructures - Part II of IV

2:30 PM-4:30 PM

Room:Society Hill Ballroom E

For Part 1 see MS70 For Part 3 see MS90

The focus of the interdisciplinary minisymposium is on continuum and discrete models of growth, patterning and formation of thin solid films and structures, as well as on analytical and numerical methods that drive such models. The speakers will describe their recent research that highlights the combination of experiment and theory, and includes such diverse phenomena as coarsening, de-wetting, directed selforganization, and phase transitions.

Organizer: Mikhail V. Khenner Western Kentucky University, USA

Organizer: Stephen J. Watson University of Glasgow, Scotland, United Kingdom

2:30-2:55 Stability and Dewetting of Metal Thin Films on Semiconductor Substrates: Clarifying the Role of Quantum Size Effect

Mikhail V. Khenner, Western Kentucky University, USA

3:00-3:25 Self-Assembled Nanoscale Patterns Produced by Ion Bombardment of Solid Surfaces

R. Mark Bradley, Colorado State University, USA

3:30-3:55 External-Field-Driven Stabilization and Patterning of Materials Surfaces

Dimitrios Maroudas, University of Massachusetts, Amherst, USA

4:00-4:25 Optimal Estimates on Contact Line Propagation for the Thin-Film Equation

Julian Fischer, Max Planck Institute for Mathematics in the Sciences, Germany Tuesday, May 10

MS81

Inverse Problems in Materials Science - Part II of IV

2:30 PM-4:30 PM

Room:Society Hill Ballroom A1

For Part 1 see MS71 For Part 3 see MS91

This minisymposium focuses on inverse problems arising in estimating the constitutive parameters of a material (e.g. its conductivity) from indirect measurements (e.g. the voltage and current on the boundary of the material). Inverse problems have many applications such as nondestructive testing, medical imaging, and climate change. The goal of this minisymposium is to highlight a broad spectrum of research results on applications of inverse problems to material sciences.

Organizer: Andrew E. Thaler Institute for Mathematics and its Applications, USA

Organizer: Fernando Guevara Vasquez

University of Utah, USA

Organizer: Maxence Cassier University of Utah, USA

2:30-2:55 Inverse Problems for Sea Ice Kenneth M. Golden, University of Utah, USA

3:00-3:25 Homogenization of a Transmission Problem

Shari Moskow, Drexel University, USA

3:30-3:55 Time Domain Inverse Problem for Maxwell's Equations in Microstructured Media

Elena Cherkaev, University of Utah, USA; Niklas Wellander, Swedish Defense Research Agency, Sweden; Dali Zhang, University of Calgary, Canada

4:00-4:25 Exact Determination of the Volume of An Inclusion in a Body with Constant Shear Modulus

Andrew E. Thaler, Institute for Mathematics and its Applications, USA; Graeme W. Milton, University of Utah, USA

Tuesday, May 10

MS82

Multiscale Behaviour of Deterministic and Probabilistic Material Models - Part II of III

2:30 PM-4:00 PM

Room:Society Hill Ballroom A2

For Part 1 see MS72 For Part 3 see MS92

This minisymposium addresses new results in the application of variational multiscale methods to systems related to materials science. We will discuss recent progress on coupling atomistic scales with continuum scales. Our main focus will be the statics and dynamics of defects such as dislocations.

Organizer: Florian Theil University of Warwick, United Kingdom

Organizer: Mark Peletier Technische Universiteit Eindhoven, The Netherlands

2:30-2:55 Temperature and Thermal Transport in Defect Kinetics: Thermomechanical Analysis of Phase Transformations in an Atomic Chain Kaushik Dayal, Carnegie Mellon

Kaushik Dayal, Carnegie Mellor University, USA

3:00-3:25 Entropy Production and Microstructure Evolution in Materials

Celia Reina, University of Pennsylvania, USA; Johannes Zimmer, University of Bath, United Kingdom

3:30-3:55 Averaging Evolving Dislocation Systems with De Rham Currents

Thomas Hochrainer, Universität Bremen, Germany

MS83

Mathematical and Computational Aspects of Nonlocal Models in Materials Science - Part IV of V

2:30 PM-4:30 PM

Room:Cook

For Part 3 see MS73 For Part 5 see MS93

The minisymposium is focused on the recent developments of nonlocal mathematical models arising in peridynamics, dynamics of complex fluid and porous media. These nonlocal models aim to quantitatively and consistently incorporate the effect of subscale phenomena such as discrete particles, cracks, polymeric molecules and microstructure into the continuum model. The talks will address both the analytical and numerical aspects of these models and their implication in our understanding of the behaviors of these materials.

Organizer: Miao-Jung Y. Ou University of Delaware, USA

Organizer: Silvia Jimenez Bolanos *Colgate University, USA*

Organizer: Bacim Alali Kansas State University, USA

2:30-2:55 Material Interfaces and Boundary Conditions in Nonlocal Diffusion.

Bacim Alali, Kansas State University, USA

3:00-3:25 Multiscale Finite Elements for Nonlocal Materials Models and Local-Nonlocal Coupling.

Timothy Costa, Oregon State University, USA; Stephen D. Bond and David Littlewood, Sandia National Laboratories, USA

3:30-3:55 A Trace Theorem for a Class of Nonlocal Energy Spaces

Xiaochuan Tian and Qiang Du, Columbia University, USA

4:00-4:25 Mathematical and Numerical Analysis for Nonlocal Parabolic Equations

Zhi Zhou, Qiang Du, and Jiang Yang, Columbia University, USA

Tuesday, May 10

MS84

Multiscale Modeling Methods for Complex Fluids and Soft Matter - Part II of III

2:30 PM-4:30 PM

Room:Flower

For Part 1 see MS74 For Part 3 see MS94

This minisymposium focuses on multiscale methods for modeling complex fluids and soft matter by concurrent coupling of macroscopic descriptions and microscopic or mesoscopic dynamics. It will include talks on theory, algorithms and diverse applications of various multiscale methods, such as, domain decomposition method, heterogeneous multiscale method, multiscale finite element/volume method, adaptive resolution scheme, multi-fidelity information fusion and others. With increasing attention on energy materials, bio-inspired materials and material assembly research, this minisymposium will bring together the researchers working on multiscale modeling to share insights and to discuss progress of key challenges in this field.

Organizer: Xin Bian Brown University, USA

Organizer: Wenxiao Pan Pacific Northwest National Laboratory, USA

2:30-2:55 Transport in Porous Electrodes Using a Multiscale Modeling Approach

W. Pan, Pacific Northwest National Laboratory, USA

3:00-3:25 Hybrid Multiscale Finite Volume Method for Advection-Diffusion-Reaction Equations

David A. Barajas-Solano and Alexander Tartakovsky, Pacific Northwest National Laboratory, USA

3:30-3:55 Parameter Inference Via Multi-Fidelity Information Fusion

Paris Perdikaris, Massachusetts Institute of Technology, USA; George E. Karniadakis, Brown University, USA

4:00-4:25 Time-Scale Bridging in Coagulation Cascade and Blood Clotting Simulations Through a Multifidelity Algorithm

Alireza Yazdani and George E. Karniadakis, Brown University, USA

continued in next column

MS85 Computational Methods for Materials Science - Part II of II

2:30 PM-5:00 PM

Room:Bromley

54

For Part 1 see MS75

The objective of the minisymposium is to bring together researchers in the field of computational material sciences and to review recent advances in this field. Various topics will be covered in the presentations: numerical methods for ab-initio calculations, resolution of multiscale partial differential equations, umbrella sampling, diffusion molecular dynamics, as well as replica-exchange free energy calculations.

Organizer: David Aristoff Colorado State University, USA

Organizer: Olivier Pinaud Colorado State University, USA

2:30-2:55 Title Not Available

Nawaf Bou-Rabee, Rutgers University, Camden, USA

3:00-3:25 Stochastic Processes and Diffusive Molecular Dynamics

Brittan A. Farmer and Mitchell Luskin, University of Minnesota, USA; Petr Plechac, University of Delaware, USA; *Gideon Simpson*, Drexel University, USA; David J. Srolovitz, University of Pennsylvania, USA

3:30-3:55 Analysis and Optimization of Stratified Sampling

Brian Van Koten, Aaron Dinner, Jeremy Tempkin, Erik Thiede, and Jonathan Weare, University of Chicago, USA

4:00-4:25 Unpacking the Thermodynamics of Small Molecule Adsorption on Nanomaterial Surfaces

Jeffrey Comer, Ran Chen, Horacio Poblete, Ariela Vergara-Jaque, and Jim Riviere, Kansas State University, USA

4:30-4:55 Information Theoretic Fitting for Coarse-Grained Molecular Dynamics

Matthew Dobson, University of Massachusetts, Amherst, USA

Tuesday, May 10

MS86 Nonlinear Waves in Lattices -Part II of III 2:30 PM-4:30 PM

Room:Claypoole

For Part 1 see MS76 For Part 3 see MS96

Many problems in materials science concern phenomena where the interplay between discreteness and nonlinearity of the medium leads to the formation of nonlinear waves. Examples include emergence of localized excitations in metamaterials and defect propagation in crystal lattices. This minisymposium features presentations of recent theoretical and experimental results by leading experts in nonlinear lattice dynamics, with an emphasis on promising mathematical developments and novel applications in materials science. It aims to facilitate a fruitful exchange of ideas among mathematicians, physicists and engineers working in this field and identify future directions and open problems.

Organizer: Anna Vainchtein University of Pittsburgh, USA

Organizer: Yuli Starosvetsky Technion - Israel Institute of Technology, Israel

2:30-2:55 Solitary Waves in the Burridge-Knopoff Model

Guillaume James, Inria Grenoble, France; Jose Eduardo Morales Morales and Arnaud Tonnelier, Inria Rhone, France

3:00-3:25 Asymptotic Formulas for Lattice Waves in the High-Energy Limit

Michael Herrmann, Universität Münster, Germany; Karsten Matthies, University of Bath, United Kingdom

3:30-3:55 Traveling Waves in Lattices with Obstacles

Aaron Hoffman, Franklin W. Olin College of Engineering, USA; Hermen Jan Hupkes, University of Leiden, The Netherlands; Erik Van Vleck, University of Kansas, USA

continued in next column

Timothy Faver, Shari Moskow, and Ronald Perline, Drexel University, USA; Yuli Starosvetsky, Technion -Israel Institute of Technology, Israel; Anna Vainchtein, University of Pittsburgh, USA; *Doug Wright*, Drexel University, USA

Coffee Break

4:30 PM-5:00 PM



Room:Hamilton Room

MS87 Metamaterials and Their Recent Applications -Part V of V

5:00 PM-7:00 PM

Room:Society Hill Ballroom B

For Part 4 see MS77

Metamaterials are materials engineered to have properties that have not yet been found in nature. This minisymposium is devoted to recent progress on understanding properties of these materials and their applications. In this minisymposium, the speakers will discuss various types of metamaterials for instance negative index materials, hyperbolic metamaterials, and seismic metamaterials and their applications such as superlensing, cloaking, cloaking via anomalous localized resonance. Different aspects of these materials such as resonance, localized resonance, stability, outgoing conditions, limiting amplitude principle are presented. Both theoretical and numerical aspects are covered.

Organizer: Hoai-Minh Nguyen École Polytechnique Fédérale de Lausanne, Switzerland

5:00-5:25 Parity-Time Symmetric Metasurfaces

Andrea Alu, University of Texas at Austin, USA

5:30-5:55 Imaging of Chiral Gratings in Inverse Electromagnetic Scattering Dinh Liem Nguyen, University of Michigan, Ann Arbor, USA

6:00-6:25 Perfectly Matched Layers for Dispersive Media and Application to Time-Domain Simulations in Metamaterials

Valentin Vinoles, Eliane Bécache, and Patrick Joly, ENSTA ParisTech, France

6:30-6:55 Numerical Simulation of Wave Propagation in Advanced Materials and Structures

Mihhail Berezovski, Embry-Riddle Aeronautical University, USA

Tuesday, May 10

MS88

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part II of VII

5:00 PM-7:00 PM

Room:Society Hill Ballroom C

For Part 1 see MS78 For Part 3 see MS98

Colloidal nematic liquid crystals arise in a host of new applications including electrophoresis, microfluidic and display devices. Chromonic liquid crystals offer new perspectives and modeling tools in biology, e.g., in studies of DNA encapsulation. Both areas add new perspectives and challenges across liquid crystal research, including newly observed defect structures and novel liquid crystal flow problems. This minisymposium will focus on understanding of defects, flows with charged particles, mechanical properties of encapsulated anisotropic systems, as well as other related problems. The minisymposium will bring together physicists, mathematicians, and biologists who will discuss their recent work encompassing experiments, modeling, and analysis

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Maria-Carme Calderer University of Minnesota, USA

Organizer: Oleg Lavrentovich Kent State University, USA

5:00-5:25 Minimizers of the Landau-de Gennes Energy Around a Spherical Colloid Particle

Lia Bronsard and Stan Alama, McMaster University, Canada; Lamy Xavier, Max Planck Institute for Mathematics in the Sciences, Germany

5:30-5:55 Optimizing Inclusions in Nematic Domains with the Ericksen Model

Shawn W. Walker, Louisiana State University, USA

6:00-6:25 Sharp-edged Colloidal Particles: Kinked Nematic Disclinations and Shape-tunable Assembly Behavior

Daniel Beller, Harvard University, USA; Mohamed Gharbi, McGill University, Canada; Iris Liu, University of Pennsylvania, USA

6:30-6:55 Magnetic Nematic Colloids

Martin Copic, University of Ljubljana, Slovenia

MS89

Efficient Numerical Methods and Analytical Techniques for Defect Problems -Part III of V

5:00 PM-7:00 PM

Room:Society Hill Ballroom D

For Part 2 see MS79 For Part 4 see MS99

Defects in crystalline materials, such as vacancies, dislocations, cracks, grain boundaries and surfaces, play important roles in the mechanical, electronic, and plastic properties of these materials. The complexity of the microstructures of these defects and their evolution at various length and time scales presents new challenges for numerical simulations and analytical modeling. The speakers in this minisymposium will discuss recent advances in the aspects of efficient numerical methods and analytical techniques as well as the obtained new findings for these defect problems.

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

5:00-5:25 Elastic Interactions and Rare Events in Irradiated Materials

Daniel Mason, Culham Centre For Fusion Energy, United Kingdom; Xiaoou Yi, Oxford University, United Kingdom; Andrea Sand, University of Helsinki, Finland; Mark Kirk, Argonne National Laboratory, USA; Sergei Dudarev, University of Oxford and Culham Centre for Fusion Energy, United Kingdom

5:30-5:55 Dislocation Climb in Discrete Dislocation Dynamics

Yejun Gu and Yang Xiang, Hong Kong University of Science and Technology, Hong Kong; David J. Srolovitz, University of Pennsylvania, USA

6:00-6:25 Second Kind Integral Equation Formulation for Dislocation Climbs in Two Dimensions

Shidong Jiang, New Jersey Institute of Technology, USA; Manas N. Rachh, Yale University, USA; Yang Xiang, Hong Kong University of Science and Technology, Hong Kong

6:30-6:55 An Efficient Level-let Model for Grain Growth Customized for Supercomputers

Christian Mießen, Nikola Velinov, Markus Kühbach, Luis-Antonio Barrales-Mora, and Günter Gottstein, RWTH Aachen University, Germany

Tuesday, May 10

MS90

Growth, Instabilities and Evolutions of Thin Films and Micro/Nanostructures -Part III of IV

5:00 PM-7:00 PM

Room:Society Hill Ballroom E

For Part 2 see MS80 For Part 4 see MS100

The focus of the interdisciplinary minisymposium is on continuum and discrete models of growth, patterning and formation of thin solid films and structures, as well as on analytical and numerical methods that drive such models. The speakers will describe their recent research that highlights the combination of experiment and theory, and includes such diverse phenomena as coarsening, de-wetting, directed selforganization, and phase transitions.

Organizer: Mikhail V. Khenner Western Kentucky University, USA

Organizer: Stephen J. Watson University of Glasgow, Scotland, United Kingdom

5:00-5:25 Corner Wetting During the Vapor-Liquid-Solid Growth of Faceted Nanowires

Brian J. Spencer, State University of New York at Buffalo, USA

5:30-5:55 Growth in Confined Environments

Oliver Pierre-Louis and Luca Gagliardi, Université Claude Bernard Lyon 1, France

6:00-6:25 The Formation and Stability of Heteroepitaxial Nanorings Simon Gill, University of Leicester,

United Kingdom

6:30-6:55 Virtually Defect Free Nanoscale Ripples Produced by Ion Bombardment of Rotating Solid Surfaces

Matt P. Harrison and Mark Bradley, Colorado State University, USA

MS91 Inverse Problems in Materials Science - Part III of IV

5:00 PM-7:00 PM

Room:Society Hill Ballroom A1

For Part 2 see MS81 For Part 4 see MS101

This minisymposium focuses on inverse problems arising in estimating the constitutive parameters of a material (e.g. its conductivity) from indirect measurements (e.g. the voltage and current on the boundary of the material). Inverse problems have many applications such as nondestructive testing, medical imaging, and climate change. The goal of this minisymposium is to highlight a broad spectrum of research results on applications of inverse problems to material sciences.

Organizer: Andrew E. Thaler Institute for Mathematics and its Applications, USA

Organizer: Fernando Guevara Vasquez *University of Utah, USA*

Organizer: Maxence Cassier University of Utah, USA

5:00-5:25 Kirchhoff Migration without Phases

Patrick Bardsley, University of Utah, USA

5:30-5:55 Inverse Scattering Problems without the Phase Information

Hoang Loc Nguyen and Michael V. Klibanov, University of North Carolina, Charlotte, USA; Kejia Pan, Central South University, China

6:00-6:25 Imaging Polarizable Dipoles

Maxence Cassier and Fernando Guevara Vasquez, University of Utah, USA

6:30-6:55 Optimal Design for Reactive-Diffusion in Materials

Lincoln Collins and Kaushik Bhattacharya, California Institute of Technology, USA

Tuesday, May 10

MS92

Multiscale Behaviour of Deterministic and Probabilistic Material Models - Part III of III 5:00 PM-6:00 PM

5.00 PIVI-0.00 PIVI

Room:Society Hill Ballroom A2

For Part 2 see MS82

This minisymposium addresses new results in the application of variational multiscale methods to systems related to materials science. We will discuss recent progress on coupling atomistic scales with continuum scales. Our main focus will be the statics and dynamics of defects such as dislocations.

Organizer: Florian Theil University of Warwick, United Kingdom

Organizer: Mark Peletier Technische Universiteit Eindhoven, The Netherlands

5:00-5:25 Finite Temperature Behavior of Crystalline Defects in the Thermodynamic Limit

Alexander Shapeev, Skolkovo Institute of Science and Technology, Russia; Mitchell Luskin, University of Minnesota, USA

5:30-5:55 An Algorithmic Consistent Two-scale Homogenization Scheme for the Characterization of Microheterogeneous Magneto-electric Composite

Joerg Schroeder and Matthias Labusch, Universität Duisburg-Essen, Germany

Tuesday, May 10

MS93

Mathematical and Computational Aspects of Nonlocal Models in Materials Science -Part V of V

5:00 PM-6:30 PM

Room:Cook

For Part 4 see MS83

The minisymposium is focused on the recent developments of nonlocal mathematical models arising in peridynamics, dynamics of complex fluid and porous media. These nonlocal models aim to quantitatively and consistently incorporate the effect of subscale phenomena such as discrete particles, cracks, polymeric molecules and microstructure into the continuum model. The talks will address both the analytical and numerical aspects of these models and their implication in our understanding of the behaviors of these materials.

Organizer: Miao-Jung Y. Ou University of Delaware, USA

Organizer: Silvia Jimenez Bolanos *Colgate University, USA*

Organizer: Bacim Alali

Kansas State University, USA

5:00-5:25 Nonlocal Higher Order Operators and Convergence to Their Classical Counterparts

Petronela Radu and Daniel Toundykov, University of Nebraska-Lincoln, USA; Jeremy Trageser, George Washington University, USA

5:30-5:55 Using Causality in Microelectronics Modeling

Lyudmyla Barannyk, University of Idaho, USA

6:00-6:25 Numerical Verification of the Bond-Based Peridynamic Softening Model Against Classical Theory

Patrick Diehl, University of Bonn, Germany; Robert P. Lipton, Louisiana State University, USA; Marc Alexander Schweitzer, University of Bonn and Fraunhofer SCAI, Germany

MS94

Multiscale Modeling Methods for Complex Fluids and Soft Matter - Part III of III

5:00 PM-6:30 PM

Room:Flower

For Part 2 see MS84

This minisymposium focuses on multiscale methods for modeling complex fluids and soft matter by concurrent coupling of macroscopic descriptions and microscopic or mesoscopic dynamics. It will include talks on theory, algorithms and diverse applications of various multiscale methods, such as, domain decomposition method, heterogeneous multiscale method, multiscale finite element/volume method, adaptive resolution scheme, multi-fidelity information fusion and others. With increasing attention on energy materials, bio-inspired materials and material assembly research, this minisymposium will bring together the researchers working on multiscale modeling to share insights and to discuss progress of key challenges in this field.

Organizer: Xin Bian Brown University, USA

Organizer: Wenxiao Pan

Pacific Northwest National Laboratory, USA

5:00-5:25 Adaptive Dual-Resolution Simulation Methods for Soft Matter: Where From, Where To?

Raffaello Potestio, Max Planck Institute for Polymer Research, Germany

5:30-5:55 Synchronized Molecular-Dynamics Simulation via Global Heat and Momentum Transports

Shugo Yasuda, University of Hyogo, Japan; Ryoichi Yamamoto, Kyoto University, Japan

6:00-6:25 The Mesh-Particle Coupling Tool MaMiCo for Multi-Resolution Fluid Dynamics: Flexibility, Parallelism, and Multi-Instance Sampling

Philipp Neumann, Technische Universität München, Germany; X Bian, Brown University, USA Tuesday, May 10

MS95

Mathematical Challenges in Phase Diagram Calculation -Part I of II

5:00 PM-7:00 PM

Room:Bromley

For Part 2 see MS105

Phase diagrams play an important role in multicomponent materials design, where inaccurate phase information may lead to costly and even disastrous consequences. Calculation of phase boundaries is a global optimization problem that poses multiple analytical and numerical challenges. While some solutions have already been discovered through the extensive use of several existing computational software packages, there is a number of outstanding issues requiring close collaboration between mathematical and materials community. This minisymposium will bring together leading researchers working in this area with an aim of discussing recent advances in the field and sharing views on most pressing remaining challenges and promising new research directions.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Igor Griva George Mason University, USA

5:00-5:25 Exploration of Multi Phase, Multi Component Thermodynamic Spaces As Solutions to Constraint Satisfaction Problems

Ray Arroyave, Sean Gibbons, Edgar Galvan, and Richard Malak, Texas A&M University, USA

5:30-5:55 The CALPHAD Gibbs Energy Minimization Challenge

Ursula Kattner, National Institute of Standards and Technology, USA

6:00-6:25 Use of Extended Gibbs Energy Algorithms for Constrained Phase Equilibria and New Kind of Phase Diagrams"

Pertti S. Koukkari and Risto Pajarre, VTT Process Chemistry, Finland

6:30-6:55 Towards Automation of Phase Diagram Calculation

Igor Griva, Maria Emelianenko, and Jeff Snider, George Mason University, USA

Tuesday, May 10

MS96

Nonlinear Waves in Lattices -Part III of III

5:00 PM-7:00 PM

Room:Claypoole

For Part 2 see MS86

Many problems in materials science concern phenomena where the interplay between discreteness and nonlinearity of the medium leads to the formation of nonlinear waves. Examples include emergence of localized excitations in metamaterials and defect propagation in crystal lattices. This minisymposium features presentations of recent theoretical and experimental results by leading experts in nonlinear lattice dynamics, with an emphasis on promising mathematical developments and novel applications in materials science. It aims to facilitate a fruitful exchange of ideas among mathematicians, physicists and engineers working in this field and identify future directions and open problems.

Organizer: Anna Vainchtein University of Pittsburgh, USA

Organizer: Yuli Starosvetsky Technion - Israel Institute of Technology, Israel

5:00-5:25 From Noisy Signals to Solitary Wave Trains

Sourish Chakravarty and *Surajit Sen*, State University of New York at Buffalo, USA

5:30-5:55 Nonlinear Dynamics in Microscale Granular Crystals

Nicholas Boechler, University of Washington, USA

6:00-6:25 From Energy Cascades and Woodpile Chains to Disordered Media and Origami Lattices

Panayotis Kevrekidis, University of Massachusetts, USA

6:30-6:55 Nonlinear Wave Dynamics in Origami-based Mechanical Metamaterials

Hiromi Yasuda, University of Washington, USA; Christopher Chong, Bowdoin College, USA; Panayotis Kevrekidis, University of Massachusetts, USA; *Jinkyu Yang*, University of Washington, USA

Registration

7:30 AM-5:30 PM Room:Society Hill Ballroom Foyer

Remarks

8:00 AM-8:15 AM Room:Society Hill Ballroom B,C,D,E

IP8

A Study of Speed Dependent Contact Angle Hysteresis

8:15 AM-9:00 AM

Room:Society Hill Ballroom B,C,D,E

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

Xiaoping Wang Hong Kong University of Science and Technology, Hong Kong

Wednesday, May 11

IP9

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

9:00 AM-9:45 AM

Room:Society Hill Ballroom B,C,D,E

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

Reidun Twarock University of York, United Kingdom

Coffee Break

9:45 AM-10:15 AM Room:Hamilton Room



Wednesday, May 11

MS97

Mathematical and Computational Issues in Electromagnetic Materials -Part I of V

10:15 AM-12:15 PM

Room:Society Hill Ballroom B

For Part 2 see MS107

The aim of this minisymposium is to bring together researchers working on fundamental questions related to electromagnetic waves and materials and to highlight recent progress in this area. Topics of focus in this minisymposium include slow light, band gap solitons, photonics, metamaterials, and resonance.

Organizer: Aaron T. Welters Florida Institute of Technology, USA

Organizer: Robert P. Lipton Louisiana State University, USA

Organizer: Stephen P. Shipman Louisiana State University, USA

Organizer: Aaron T. Welters Florida Institute of Technology, USA

10:15-10:40 Spectral Theory with Out Ellipticity: Bloch Waves and Separation of Frequency Spectra *Robert P. Lipton* and Robert Viator Jr.,

Louisiana State University, USA

10:45-11:10 Efficient Solvers for Electromagnetic Wave Propagation Problems in Complex Geometries *Catalin Turc*, New Jersey Institute of

Technology, USA

11:15-11:40 Gap Solitons in Almost Periodic One-Dimensional Structures Alexander Pankov, Morgan State University, USA

11:45-12:10 Boundary Value Problems for the Anistropic Maxwell System in Lipschitz Domains

Eric Stachura, Temple University, USA

MS98

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part III of VII

10:15 AM-12:15 PM

Room:Society Hill Ballroom C

For Part 2 see MS88 For Part 4 see MS108

Colloidal nematic liquid crystals arise in a host of new applications including electrophoresis, microfluidic and display devices. Chromonic liquid crystals offer new perspectives and modeling tools in biology, e.g., in studies of DNA encapsulation. Both areas add new perspectives and challenges across liquid crystal research, including newly observed defect structures and novel liquid crystal flow problems. This minisymposium will focus on understanding of defects, flows with charged particles, mechanical properties of encapsulated anisotropic systems, as well as other related problems. The minisymposium will bring together physicists, mathematicians, and biologists who will discuss their recent work encompassing experiments, modeling, and analysis

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Maria-Carme Calderer University of Minnesota, USA

Organizer: Oleg Lavrentovich Kent State University, USA

10:15-10:40 Point Defects in the Landau-de Gennes Model: Qualitative Features and Stability

Arghir Zarnescu, University of Sussex, United Kingdom

10:45-11:10 On Weak Anchoring for a Two-Dimensional Nematic Liquid Crystal

Stan Alama and Lia Bronsard, McMaster University, Canada; Bernardo Galvao-Sousa, University of Toronto, Canada

11:15-11:40 Limits of minimizers of a Landau-de Gennes functional

Alberto Montero, Pontificia Universidad Católica de Chile, Chile; Dmitry Golovaty, University of Akron, USA

11:45-12:10 Geometrically Nonlinear Models for Nematic Elastomers

Marco Barchiesi, Università degli Studi di Napoli Federico II, Italy; *Duvan Henao*, Pontificia Universidad Católica de Chile, Chile; Carlos Mora-Corral, Universidad Autonoma de Madrid, Spain

Wednesday, May 11 MS99

Efficient Numerical Methods and Analytical Techniques for Defect Problems -Part IV of V

10:15 AM-12:15 PM

Room:Society Hill Ballroom D

For Part 3 see MS89 For Part 5 see MS109

Defects in crystalline materials, such as vacancies, dislocations, cracks, grain boundaries and surfaces, play important roles in the mechanical, electronic, and plastic properties of these materials. The complexity of the microstructures of these defects and their evolution at various length and time scales presents new challenges for numerical simulations and analytical modeling. The speakers in this minisymposium will discuss recent advances in the aspects of efficient numerical methods and analytical techniques as well as the obtained new findings for these defect problems.

Organizer: Yang Xiang

Hong Kong University of Science and Technology, Hong Kong

10:15-10:40 Quantized Vortex Dynamics and Interaction in Superfluidity and Superconductivity on Bounded Domains

Weizhu Bao, National University of Singapore, Singapore

10:45-11:10 Multiscale Model for Interlayer Dislocations in Bilayer Graphene

Shuyang Dai, University of Pennsylvania, USA; Yang Xiang, Hong Kong University of Science and Technology, Hong Kong; David J. Srolovitz, University of Pennsylvania, USA

11:15-11:40 Blended Atomisticto-Continuum Hybrid Methods for Modeling Crystalline Materials

Xingjie Li, University of North Carolina, Charlotte, USA; Brian Van Koten, University of Chicago, USA; Mitchell Luskin and Derek Olson, University of Minnesota, USA; Christoph Ortner, University of Warwick, United Kingdom; Alexander Shapeev, Skolkovo Institute of Science and Technology, Russia

11:45-12:10 Mathematical Modeling and Analysis of Plasmonic Nanoparticles

Hai Zhang, Hong Kong University of Science and Technology, Hong Kong

Wednesday, May 11

MS100

Growth, Instabilities and Evolutions of Thin Films and Micro/Nanostructures -Part IV of IV

10:15 AM-11:15 AM

Room:Society Hill Ballroom E

For Part 3 see MS90

The focus of the interdisciplinary minisymposium is on continuum and discrete models of growth, patterning and formation of thin solid films and structures, as well as on analytical and numerical methods that drive such models. The speakers will describe their recent research that highlights the combination of experiment and theory, and includes such diverse phenomena as coarsening, de-wetting, directed selforganization, and phase transitions.

Organizer: Mikhail V. Khenner Western Kentucky University, USA

Organizer: Stephen J. Watson University of Glasgow, Scotland, UK

10:15-10:40 Producing Nanodot Arrays with Improved Hexagonal Order by Patterning Surfaces Before Ion Sputtering

Daniel A. Pearson and Richard Bradley, Colorado State University, USA; Francis Motta, Duke University, USA; Patrick Shipman, Colorado State University, USA

10:45-11:10 Asymmetric Shape Transitions of Epitaxial Quantum Dots from Pyramid to Multifaceted Dome

Chaozhen Wei and Brian J. Spencer, State University of New York at Buffalo, USA

Wednesday, May 11

Inverse Problems in Materials Science -Part IV of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom A1

For Part 3 see MS91

This minisymposium focuses on inverse problems arising in estimating the constitutive parameters of a material (e.g. its conductivity) from indirect measurements (e.g. the voltage and current on the boundary of the material). Inverse problems have many applications such as nondestructive testing, medical imaging, and climate change. The goal of this minisymposium is to highlight a broad spectrum of research results on applications of inverse problems to material sciences.

Organizer: Andrew E. Thaler Institute for Mathematics and its Applications, USA

Organizer: Fernando Guevara Vasquez

University of Utah, USA

Organizer: Maxence Cassier University of Utah, USA

10:15-10:40 Active Control for the Helmholtz Equation by Almost Non-Radiating Solutions

Mark Hubenthal, Institute for Mathematics and its Applications, USA; Daniel Onofrei, University of Houston, USA

10:45-11:10 Model Order Reduction in Inverse Problem for Maxwell's Equations

Michal A. Kordy, Elena Cherkaev, and Phil Wannamaker, University of Utah, USA

MS101 Inverse Problems in Materials Science -Part IV of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom A1 continued

11:15-11:40 Nonlinear Imaging with Waves via Model Order Reduction

Alexander V. Mamonov, University of Houston, USA; Vladimir L. Druskin, Schlumberger-Doll Research, USA; Andrew E. Thaler, Institute for Mathematics and its Applications, USA; Mikhail Zaslavsky, Schlumberger-Doll Research, USA

11:45-12:10 On the Discreteness of the Interior Transmission Eigenvalues

Hoai-Minh Nguyen and Quoc Hung Nguyen, École Polytechnique Fédérale de Lausanne, Switzerland Wednesday, May 11

MS102

Particle-Based Methods for Modeling Materials -Part I of II

10:15 AM-12:15 PM

Room:Society Hill Ballroom A2

For Part 2 see MS112

This minisymposium focuses on particlebased methods for modeling materials including soft matters, energy materials and bio-inspired materials. It will include talks on theory, algorithms and diverse applications of moving least square (MLS), smoothed particle hydrodynamics (SPH), radial basis functions (RBF), dissipative particle dynamics (DPD), and other particle-based methods. Particlebased methods have advantages for modeling physical phenomena involving large-deformation of materials, moving interfaces in multiphase complex fluids, advection-dominated transport, etc. This minisymposium will bring together researchers working on particle-based methods to share insights and to discuss progress of key challenges in this field and promote discussion of similarities between methods.

Organizer: Wenxiao Pan Pacific Northwest National Laboratory, USA

Organizer: Nathaniel Trask Brown University, USA

10:15-10:40 Fundamental Studies of Dynamic Fracture with Multiscale Peridynamics

Stewart Silling, Sandia National Laboratories, USA

10:45-11:10 A Monolithic Compatible Meshless Discretization for Simulating Electrophoretic Suspensions Nathaniel Trask, Brown University, USA

11:15-11:40 Radial Basis Function Methods for Meshfree Transport on the Sphere and Other Surfaces

Varun Shankar, University of Utah, USA; Grady B. Wright, Boise State University, USA

11:45-12:10 Practices of Coarse-Graining Based on the Mori-Zwanzig Formalism

Zhen Li and Xin Bian, Brown University, USA; Xiantao Li, Pennsylvania State University, USA; George Em Karniadakis, Brown University, USA

continued in next column

MS103

Microscopic, Mesoscale and Macroscale Models in Mechanics - Part I of II

10:15 AM-12:15 PM

Room:Cook

For Part 2 see MS113

A variety of important physical processes involve the interaction of atomistic, mesoscopic and macroscopic scales. For example, in materials science, defects are often described by invoking atomistic, mesoscale or fully continuum principles of mechanics. The development of viable theories for such physical phenomena can be challenging, touching upon issues of modeling, scientific computation and mathematical analysis in deterministic or stochastic settings. The purpose of this minisymposium is to bring together researchers who work in diverse fields of mechanics with emphasis on understanding the synergy of different scales, from the atomistic to the full continuum.

Organizer: Jianfeng Lu Duke University, USA

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

10:15-10:40 Second Order Gamma-Convergence for the Modica Mortola Functional

Irene Fonseca, Carnegie Mellon University, USA

10:45-11:10 Variational Convergence for the Analysis of Boundary Layers in Dislocation Pileups

Patrick Van Meurs, Kanazawa University, Japan; Adriana Garroni, Universita di Roma "La Sapienza," Italy; Mark Peletier, Technische Universiteit Eindhoven, The Netherlands; Lucia Scardia, University of Bath, United Kingdom

11:15-11:40 A Continuum Model for Dislocation Dynamics in Three Dimensions Using the Dislocation Density Potential Functions

Yang Xiang and Yichao Zhu, Hong Kong University of Science and Technology, Hong Kong

11:45-12:10 Seamless Coupling of Nonlocal and Local Models

Qiang Du, Yunzhe Tao, and Xiaochuan Tian, Columbia University, USA

Wednesday, May 11

MS104

Soft Elastic Materials: Nonlinear Constitutive Models, Mathematical and Mechanical Aspects -Part I of III

10:15 AM-12:15 PM

Room:Flower

For Part 2 see MS114

Soft materials like rubber of soft biological tissues are subject to large elastic deformations. Anisotropy and other nonlinear effects in such materials leads to complex nonlinear models. The objective of the Minisymposium is to provide an overview of up-to-date research in the field and foster further interdisciplinary collaborations, through the consideration of both mechanical and mathematical aspects. The following topics will be addressed:

- Advances in theoretical approaches
- Symmetry analysis of BVPs in nonlinear elasticity
- Exact solutions
- Numerical aspects
- Formulation and identification of constitutive models
- Wave propagation aspects
- Applications to soft biological tissues (arteries, biomembranes)
- Stability issues

Organizer: Alexei F. Cheviakov University of Saskatchewan, Canada

Organizer: Jean-François Ganghoffer

LEMTA, Université de Lorraine, France

10:15-10:40 Nonclassical Analysis of the Nonlinear Kompaneets Equation *George Bluman*, University of British Columbia, Canada

MS104

Soft Elastic Materials: Nonlinear Constitutive Models, Mathematical and Mechanical Aspects -Part I of III

10:15 AM-12:15 PM

Room:Flower

continued

10:45-11:10 Nonlinear Elastodynamic Models of Wave Propagation and Conservation Laws for Fiber-Reinforced Materials

Alexei F. Cheviakov, University of Saskatchewan, Canada

11:15-11:40 Computation of the Effective Nonlinear Mechanical Response of Lattice Materials Considering Internal Scale Effects

Jean-François Ganghoffer, LEMTA, Université de Lorraine, France

11:45-12:10 Geometry of Thin Nematic Elastomer Sheets

Hillel Aharoni, University of Pennsylvania, USA; Eran Sharon and Raz Kupferman, Hebrew University of Jerusalem, Israel Wednesday, May 11

MS105

Mathematical Challenges in Phase Diagram Calculation -Part II of II

10:15 AM-11:15 AM

Room:Bromley

For Part 1 see MS95

Phase diagrams play an important role in multicomponent materials design, where inaccurate phase information may lead to costly and even disastrous consequences. Calculation of phase boundaries is a global optimization problem that poses multiple analytical and numerical challenges. While some solutions have already been discovered through the extensive use of several existing computational software packages, there is a number of outstanding issues requiring close collaboration between mathematical and materials community. This minisymposium will bring together leading researchers working in this area with an aim of discussing recent advances in the field and sharing views on most pressing remaining challenges and promising new research directions.

Organizer: Maria Emelianenko George Mason University, USA

Organizer: Igor Griva George Mason University, USA

10:15-10:40 Numerical Challenges in Computing Thermodynamic Equilibria in Large Complex Systems and Upon Integration in Multi-Physics Codes

Markus Piro, Canadian Nuclear Laboratories, Canada; Srdjan Simunovic, Oak Ridge National Laboratory, USA

10:45-11:10 Global Energy Minimization of Multi-Component Phases with Internal Degrees of Freedom

Richard Otis, Pennsylvania State University, USA

Wednesday, May 11

MS106

Mechanics, Electro- and Hydro- dynamics of Drops and Vesicles - Part I of III

10:15 AM-12:15 PM

Room:Claypoole

For Part 2 see MS116

Drops and vesicles (self-enclosing unilamellar lipid bilayer) are ubiquitous in material sciences as their mechanics and dynamics are relevant to a wide range of engineering applications. Vesicles are used as biomimetic model membranes to shed light on how cell membranes uptake nano-particles and remodel under forces. The electrohydrodynamics of particles on the drop surface is investigated to understand how charged macromolecules transport on membranes. This minisymposium brings together experts in different aspects of this field to discuss new discoveries and novel mathematics for modeling the complex mechanics and dynamics of drops and vesicles as they interact with particles, charges and fluid in the context of biological soft materials.

Organizer: Yuan-Nan Young New Jersey Institute of Technology, USA

10:15-10:40 Simulations of Particle Structuring Driven by Electric Fields

Michael Miksis and Yi Hu, Northwestern University, USA; Petia Vlahovska, Brown University, USA

10:45-11:10 Dynamics and Thermal Fluctuations of Particles On/Near an Interface

Paul Salipante, National Institute of Standards and Technology, USA

11:15-11:40 A Molecular Dynamics Study on the Mechanics of the Lipid Bilayer Membrane Containing an Integrin Protein under Shock Loading. *Ralph Kfoury* and Hongyan Yuan,

University of Rhode Island, USA

11:45-12:10 Mechanics of Cell Interaction with Two-Dimensional Nanomaterials

Xin Yi, Brown University, USA

Lunch Break 12:15 PM-1:30 PM Attendees on their own

IP10

Title Not Available

1:30 PM-2:15 PM Room:Society Hill Ballroom B,C,D,E Abstract not available at time of publication.

Christof Schütte Freie Universität Berlin, Germany

Intermission

2:15 PM-2:30 PM

Wednesday, May 11

MS107

Mathematical and Computational Issues in Electromagnetic Materials -Part II of V

2:30 PM-4:30 PM

Room:Society Hill Ballroom B

For Part 1 see MS97 For Part 3 see MS117 The aim of this minisymposium is to bring together researchers working on fundamental questions related to electromagnetic waves and materials and to highlight recent progress in this area. Topics of focus in this minisymposium include slow light, band gap solitons, photonics, metamaterials, and resonance.

Organizer: Aaron T. Welters Florida Institute of Technology, USA

Organizer: Robert P. Lipton Louisiana State University, USA

Organizer: Stephen P. Shipman Louisiana State University, USA

Organizer: Aaron T. Welters Florida Institute of Technology, USA

2:30-2:55 Soliton Solutions of the Nonlinear Exciton-Polariton Equations Stephen P. Shipman, Louisiana State University, USA

3:00-3:25 Existence and Stability Properties of Radial Bound States for Schrödinger-Poisson Equation with external Coulomb potential in Three Space Dimensions

Jeremy L. Marzuola, University of North Carolina at Chapel Hill, USA; Sarah Raynor, Wake Forest University, USA; *Gideon Simpson*, Drexel University, USA

3:30-3:55 Quantum Optics in Random Media

John Schotland, University of Michigan, USA

4:00-4:25 Weak Wave Turbulence in Systems with PT-Symmetry.

Alexey Sukhinin, Southern Methodist University, USA

Wednesday, May 11

MS108

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part IV of VII

2:30 PM-4:30 PM

Room:Society Hill Ballroom C

For Part 3 see MS98 For Part 5 see MS118

Colloidal nematic liquid crystals arise in a host of new applications including electrophoresis, microfluidic and display devices. Chromonic liquid crystals offer new perspectives and modeling tools in biology, e.g., in studies of DNA encapsulation. Both areas add new perspectives and challenges across liquid crystal research, including newly observed defect structures and novel liquid crystal flow problems. This minisymposium will focus on understanding of defects, flows with charged particles, mechanical properties of encapsulated anisotropic systems, as well as other related problems. The minisymposium will bring together physicists, mathematicians, and biologists who will discuss their recent work encompassing experiments, modeling, and analysis

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Maria-Carme Calderer

University of Minnesota, USA

Organizer: Oleg Lavrentovich Kent State University, USA

2:30-2:55 Mathematical Descriptions of Point, Line and Surface Defects John Ball and Stephen Bedford,

University of Oxford, United Kingdom

MS108

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part IV of VII

2:30 PM-4:30 PM

Room:Society Hill Ballroom C

continued

3:00-3:25 Limiting Behaviors of Bent-Core Liquid Crystal Models

Tiziana Giorgi, New Mexico State University, USA; Sookyung Joo, Old Dominion University, USA; Carlos J. Garcia-Cerver, University of California, Santa Barbara, USA

3:30-3:55 Dimension Reduction for the Landau-de Gennes Model of Nematic Films on Surfaces

Dmitry Golovaty, University of Akron, USA; Peter Sternberg, Indiana University, USA; Alberto Montero, Pontificia Universidad Católica de Chile, Chile

4:00-4:25 A Topological Obstruction Related to Nematic Shells: Morse's Index Formula for VMO Vector Fields

Giacomo Canevari, University of Oxford, United Kingdom and Pierre and Marie Curie University, France Wednesday, May 11

MS109

Efficient Numerical Methods and Analytical Techniques for Defect Problems - Part V of V

2:30 PM-4:30 PM

Room:Society Hill Ballroom D

For Part 4 see MS99

Defects in crystalline materials, such as vacancies, dislocations, cracks, grain boundaries and surfaces, play important roles in the mechanical, electronic, and plastic properties of these materials. The complexity of the microstructures of these defects and their evolution at various length and time scales presents new challenges for numerical simulations and analytical modeling. The speakers in this minisymposium will discuss recent advances in the aspects of efficient numerical methods and analytical techniques as well as the obtained new findings for these defect problems.

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

2:30-2:55 Efficient Algorithms for Transition State Calculations Weiguo Gao, Fudan University, China

3:00-3:25 Grain Boundary Roughening in Colloidal Crystals

Yilong Han, Hong Kong University of Science and Technology, Hong Kong

3:30-3:55 Grain Boundary Migration in Nanocrystalline Metals

Spencer L. Thomas and David J. Srolovitz, University of Pennsylvania, USA

4:00-4:25 A Continuum Model for Dynamics of Dislocation Arrays and Applications to Low Angle Grain Boundaries

Luchan Zhang and Yejun Gu, Hong Kong University of Science and Technology, Hong Kong; Xiaohong Zhu, Jinan University, China; Yang Xiang, Hong Kong University of Science and Technology, Hong Kong

Wednesday, May 11

MS110

Wetting/Dewetting in Complex Fluids and Thin Solid Films - Part I of IV

2:30 PM-4:30 PM

Room:Society Hill Ballroom E

For Part 2 see MS120

Tremendous progress has been achieved in recent years on wetting/ dewetting problems in complex fluids and thin solid films, such as complex wetting phenomena on liquids, solidstate dewetting of thin films and moving contact lines dynamics. This minisymposium aims to promote interdisciplinary research collaborations among applied and computational mathematicians, and material scientists. Active experts and research groups in this field will deliver their thoughts and experiences on topics of wetting/ dewetting from applied and computational mathematics, theoretical and experimental materials sciences, and discuss recent developments, possible collaborations and exciting future directions in the field of wetting/dewetting.

Organizer: Weizhu Bao

National University of Singapore, Singapore

Organizer: Wei Jiang Wuhan University, China

2:30-2:55 Instabilities During Solid State Dewetting of Thin Films

Carl V. Thompson, Massachusetts Institute of Technology, USA

3:00-3:25 The Effect of Nanoindentation on Thermal Stability and Dewetting of Thin Metal Films

Eugen Rabkin, Technion - Israel Institute of Technology, Israel

3:30-3:55 Wetting in Thin Solid Polycrystalline Films

Vadim Derkach, Technion - Israel Institute of Technology, Israel; John McCuan, Georgia Institute of Technology, USA; *Amy Novick-Cohen*, Technion - Israel Institute of Technology, Israel

4:00-4:25 Kinetics of the Triple Line in Solid-State Wetting

Oliver Pierre-Louis, Université Claude Bernard Lyon 1, France

MS111 Mathematical Modeling of Microstructured Materials -Part I of IV

2:30 PM-4:30 PM

Room:Society Hill Ballroom A1

For Part 2 see MS121

The goal of the minisymposium is to discuss the latest development in the area among mathematicians, material scientists and engineers, and identify important open problems. The list of topics includes but not limited to mathematical modeling of nanomaterials and biological nano-structures, homogenization and effective properties of composite materials, anisotropic behavior of composites with arbitrarily oriented inclusions and microcracks, analytical and numerical methods in periodic and random composites, inverse problems and microelectronic modeling.

Organizer: Lyudmyla Barannyk University of Idaho, USA

Organizer: Yuri Godin University of North Carolina, Charlotte, USA

Organizer: Yuliya Gorb University of Houston, USA

Organizer: Alexander Panchenko Washington State University, USA

2:30-2:55 Surface-Elasticity-Based Approach in Modeling Material Microstructure in Fracture Problems

Anna Zemlyanova, Kansas State University, USA

3:00-3:25 Variational Principle for Probabilistic Measure in Theory of Materials with Random Microstructure

Victor Berdichevsky, Wayne State University, USA

3:30-3:55 Disordered Hyperuniform Materials: Novel States of Amorphous Matter

Salvatore Torquato, Princeton University, USA

4:00-4:25 Transport Properties of a Periodic Array of Spherical Inclusions

Yuri Godin, University of North Carolina, Charlotte, USA

Wednesday, May 11

MS112

Particle-Based Methods for Modeling Materials - Part II of II

2:30 PM-4:30 PM

Room:Society Hill Ballroom A2

For Part 1 see MS102

This minisymposium focuses on particlebased methods for modeling materials including soft matters, energy materials and bio-inspired materials. It will include talks on theory, algorithms and diverse applications of moving least square (MLS), smoothed particle hydrodynamics (SPH), radial basis functions (RBF), dissipative particle dynamics (DPD), and other particle-based methods. Particlebased methods have advantages for modeling physical phenomena involving large-deformation of materials, moving interfaces in multiphase complex fluids, advection-dominated transport, etc. This minisymposium will bring together researchers working on particle-based methods to share insights and to discuss progress of key challenges in this field and promote discussion of similarities between methods.

Organizer: Wenxiao Pan Pacific Northwest National Laboratory, USA

Organizer: Nathaniel Trask Brown University, USA

2:30-2:55 Integral Approximations to Classical Diffusion and Smoothed Particle Hydrodynamics

Richard B. Lehoucq, Sandia National Laboratories, USA

3:00-3:25 Smoothed Particle Hydrodynamics: Consistence, Convergence and Transport-Velocity Formulation

Xiangyu Hu, Technische Universität München, Germany

3:30-3:55 Simulating Transport in Microfluidics and Porous Electrodes by Implicit Incompressible Smoothed Particle Hydrodynamics

Wenxiao Pan, Pacific Northwest National Laboratory, USA; Kyungjoo Kim and Mauro Perego, Sandia National Laboratories, USA

4:00-4:25 Quantifying the Dynamics of Thermo-Responsive Polymers As Drug Delivery Vehicles

Yu-Hang Tang, Zhen Li, Xuejin Li, Mingge Deng, and George E. Karniadakis, Brown University, USA

continued in next column

MS113

Microscopic, Mesoscale and Macroscale Models in Mechanics - Part II of II

2:30 PM-4:30 PM

Room:Cook

For Part 1 see MS103

A variety of important physical processes involve the interaction of atomistic, mesoscopic and macroscopic scales. For example, in materials science, defects are often described by invoking atomistic, mesoscale or fully continuum principles of mechanics. The development of viable theories for such physical phenomena can be challenging, touching upon issues of modeling, scientific computation and mathematical analysis in deterministic or stochastic settings. The purpose of this minisymposium is to bring together researchers who work in diverse fields of mechanics with emphasis on understanding the synergy of different scales, from the atomistic to the full continuum.

Organizer: Jianfeng Lu Duke University, USA

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

2:30-2:55 Propagation of Chaos for Many Particle Systems with Diffusion in Velocity

Pierre-Emmanuel Jabin and Zhenfu Wang, University of Maryland, USA

3:00-3:25 On the Existence and Regularity of Solutions to Euler's Equations for Hard Non-Spherical Particles

Mark Wilkinson, Courant Institute of Mathematical Sciences, New York University, USA; Peter Palffy-Muhoray and Xiaoyu Zheng, Kent State University, USA

3:30-3:55 1D Static Phase Field Crystals Coupled with Continuum Elasticity

Jianfeng Lu, Duke University, USA; Benedikt Wirth, Universität Münster, Germany

4:00-4:25 Coarsening Dynamics for the Cahn-Hilliard Equation with Degenerate Mobility

Shibin Dai, New Mexico State University, USA; Qiang Du, Columbia University, USA Wednesday, May 11

MS114

Soft Elastic Materials: Nonlinear Constitutive Models, Mathematical and Mechanical Aspects -Part II of III

2:30 PM-4:00 PM

Room:Flower

For Part 1 see MS104 For Part 3 see MS124

Soft materials like rubber of soft biological tissues are subject to large elastic deformations. Anisotropy and other nonlinear effects in such materials leads to complex nonlinear models. The objective of the Minisymposium is to provide an overview of up-to-date research in the field and foster further interdisciplinary collaborations, through the consideration of both mechanical and mathematical aspects. The following topics will be addressed: - Advances in theoretical approaches - Symmetry analysis of BVPs in nonlinear elasticity - Exact solutions - Numerical aspects - Formulation and identification of constitutive models - Wave propagation aspects - Applications to soft biological tissues (arteries, biomembranes) -Stability issues

Organizer: Alexei F. Cheviakov University of Saskatchewan, Canada

Organizer: Jean-François Ganghoffer

LEMTA, Université de Lorraine, France

2:30-2:55 On the General Solution Based on the Time-Independent Integral, the Lagrangian and the Hamiltonian Functions for Fin Equation *Teoman Özer* and Özlem Orhan, Istanbul Technical University, Turkey

3:00-3:25 Multiscale Modeling of Rubber-Like Materials and Soft Tissues: *Particular Perspective*

Giuseppe Saccomandi, Università di Perugia, Italy

3:30-3:55 Conditions for the Holder Regularity of Local Minimizers of a Nonlinear Elastic Energy in Two Dimensions

Jonathan J. Bevan, University of Surrey, United Kingdom

Wednesday, May 11

MS115

Non-Equilibrium Phenomena for Liquid Crystals: Mathematical Case Studies - Part I of IV

2:30 PM-4:30 PM

Room:Bromley

For Part 2 see MS125

Liquid crystals (LCs) are partially ordered materials. The mathematics of LCs for example, the Landau-de Gennes theory, raises challenging problems across the calculus of variations, partial differential equations, geometry and numerical analysis. This minisymposium is dedicated to non-equilibrium phenomena for LCs, in a non-variational setting that abound in applications such as nematic microfluidics, active matter and bio-materials. The talks address fundamental questions such as existence and regularity of solutions, effects of curvature and multiscale LC dynamics. A large proportion of the invited speakers are from under-represented research groups in the Far East, who have made recent contributions to the field.

Organizer: Changyou Wang Purdue University, USA

Organizer: Apala Majumdar University of Bath, United Kingdom

Organizer: Pingwen Zhang Peking University, China

2:30-2:55 Solution Landscapes for Nematic Microfluidics

Ian Griffiths, University of Oxford, United Kingdom

3:00-3:25 Global Existence and Finite Time Singularities for a Simplified Model of Liquid Crystal Flows

Tao Huang, New York University-Shanghai, China

3:30-3:55 Flexible Colloidal Molecules: Lipid Ordering Regulated Bond Flexibility

Daniela J. Kraft, Leiden University, Netherlands

4:00-4:25 Linear Stability of Compressible Vortex Sheets in Elastodynamics Jilong Hu, University of Pittsburgh, USA

MS116

Mechanics, Electro- and Hydro- dynamics of Drops and Vesicles - Part II of III

2:30 PM-4:30 PM

Room:Claypoole

For Part 1 see MS106 For Part 3 see MS126

Drops and vesicles (self-enclosing unilamellar lipid bilayer) are ubiquitous in material sciences as their mechanics and dynamics are relevant to a wide range of engineering applications. Vesicles are used as biomimetic model membranes to shed light on how cell membranes uptake nano-particles and remodel under forces. The electro-hydrodynamics of particles on the drop surface is investigated to understand how charged macromolecules transport on membranes. This minisymposium brings together experts in different aspects of this field to discuss new discoveries and novel mathematics for modeling the complex mechanics and dynamics of drops and vesicles as they interact with particles, charges and fluid in the context of biological soft materials.

Organizer: Yuan-Nan Young New Jersey Institute of Technology, USA

2:30-2:55 Computational Algorithms for Vesicle Electrohydrodynamics

Shravan Veerapaneni, University of Michigan, USA

3:00-3:25 Recent Advances in Modeling of Liposomes in Electric and Magnetic Fields

David Salac and Prerna Gera, State University of New York at Buffalo, USA

3:30-3:55 A Hybrid Numerical Method for Electrokinetic Flow with Deformable Interfaces

Michael R. Booty and Michael Siegel, New Jersey Institute of Technology, USA

4:00-4:25 An Accurate Metropolis-Hastings Algorithm and a Fast Multipole Method for Coarse-Grained Lipid Bilayer Membrane in Solvent

Szu-Pei Fu and Shidong Jiang, New Jersey Institute of Technology, USA; Nawaf Bou-Rabee, Rutgers University, Camden, USA; Yuan-Nan Young, New Jersey Institute of Technology, USA; Zhangli Peng, University of Notre Dame, USA; Hongyan Yuan, University of Rhode Island, USA

Coffee Break

4:30 PM-5:00 PM Room:Hamilton Room



Wednesday, May 11

MS117

Mathematical and Computational Issues in Electromagnetic Materials -Part III of V

5:00 PM-6:30 PM

Room:Society Hill Ballroom B

For Part 2 see MS107 For Part 4 see MS127

The aim of this minisymposium is to bring together researchers working on fundamental questions related to electromagnetic waves and materials and to highlight recent progress in this area. Topics of focus in this minisymposium include slow light, band gap solitons, photonics, metamaterials, and resonance.

Organizer: Aaron T. Welters Florida Institute of Technology, USA

Organizer: Robert P. Lipton Louisiana State University, USA

Organizer: Stephen P. Shipman Louisiana State University, USA

Organizer: Aaron T. Welters Florida Institute of Technology, USA

5:00-5:25 Pathological Scattering of Electromagnetic Waves in Magneto-Photonic Crystals with Defects in the Slow-Light Regime

Aaron T. Welters, Florida Institute of Technology, USA; Shipman Shipman, Louisiana State University, USA

5:30-5:55 Highly Accurate Methods for Resonance Calculations

Nilima Nigam, Simon Fraser University, Canada

6:00-6:25 Novel Integral Formulations for Layered Media Problems in Electromagnetics

Michael O'Neil, New York University, USA

MS118

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part V of VII

5:00 PM-7:00 PM

Room:Society Hill Ballroom C

For Part 4 see MS108 For Part 6 see MS128

Colloidal nematic liquid crystals arise in a host of new applications including electrophoresis, microfluidic and display devices. Chromonic liquid crystals offer new perspectives and modeling tools in biology, e.g., in studies of DNA encapsulation. Both areas add new perspectives and challenges across liquid crystal research, including newly observed defect structures and novel liquid crystal flow problems. This minisymposium will focus on understanding of defects. flows with charged particles, mechanical properties of encapsulated anisotropic systems, as well as other related problems. The minisymposium will bring together physicists, mathematicians, and biologists who will discuss their recent work encompassing experiments, modeling, and analysis

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Maria-Carme Calderer University of Minnesota, USA

Organizer: Oleg Lavrentovich Kent State University, USA

5:00-5:25 Liquid Crystal Electrokinetics Maria-Carme Calderer, University of Minnesota, USA

5:30-5:55 Theory and Experiments of Topologically Driven Flows in Nematic Suspensions

Jorge Vinals, University of Minnesota, USA

6:00-6:25 Regularity and Related Properties for Minimizers of Maier-Saupe Energies for Liquid Crystals Patricia Bauman, Purdue University, USA

6:30-6:55 Mean Field Models for Lyotropic Nematic Liquid Crystals Mark Wilkinson, Courant Institute of Mathematical Sciences, New York University, USA

Wednesday, May 11

MS119

Multiscale Modelling and Simulations of Dislocations for Continuum Plasticity -Part I of III

5:00 PM-7:00 PM

Room:Society Hill Ballroom D

For Part 2 see MS129

This minisymposium is aimed to provide a platform for exchanging ideas over recent progress made in theoretical or computational considerations of dislocations on a multiscale basis. Attentions will be paid especially to the understanding of the connection between dislocation behaviour and continuum plasticity.

Organizer: Katrin Schulz Karlsruhe Institute of Technology, Germany

Organizer: Yichao Zhu Hong Kong University of Science and Technology, Hong Kong

5:00-5:25 On the Connection Between Dislocation Mechanics and Continuum Crystal Plasticity

Amit Acharya, Carnegie Mellon University, USA; Xiaohan Zhang, Stanford University, USA; Saurabh Puri, Dassault Systemes Simulia Corp, USA

5:30-5:55 Thermodynamically Consistent Continuum Dislocation Dynamics

Thomas Hochrainer and Alireza Ebrahimi, Universität Bremen, Germany

6:00-6:25 Capturing the Stochastic Behavior of Nanoindentation Pop-In with Dislocation Dynamics

Joshua C. Crone, Lynn B. Munday, and Jaroslaw Knap, U.S. Army Research Laboratory, USA

6:30-6:55 Free Energy Function of Dislocation Densities by Large Scale Atomistic Simulation

Christoph Begau, Ruhr-Universitat Bochum, Germany

MS120

Wetting/Dewetting in Complex Fluids and Thin Solid Films - Part II of IV

5:00 PM-7:00 PM

Room:Society Hill Ballroom E

For Part 1 see MS110 For Part 3 see MS130

Tremendous progress has been achieved in recent years on wetting/ dewetting problems in complex fluids and thin solid films, such as complex wetting phenomena on liquids, solid-state dewetting of thin films and moving contact lines dynamics. This minisymposium aims to promote interdisciplinary research collaborations among applied and computational mathematicians, and material scientists. Active experts and research groups in this field will deliver their thoughts and experiences on topics of wetting/dewetting from applied and computational mathematics, theoretical and experimental materials sciences, and discuss recent developments, possible collaborations and exciting future directions in the field of wetting/ dewetting.

Organizer: Weizhu Bao National University of Singapore, Singapore

Organizer: Wei Jiang *Wuhan University, China*

5:00-5:25 Solid State Dewetting on Curved Substrates

David J. Srolovitz, University of Pennsylvania, USA; Yan Wang, National University of Singapore, Singapore; Wei Jiang, Wuhan University, China; Weizhu Bao, National University of Singapore, Singapore

5:30-5:55 Nanostructure Formation via Template-Guided Dewetting

Yong-Wei Zhang, Liangxing Lu, and Bharathi Srinivasan, Institute of High Performance Computing, Singapore; Yingmin Wang, Mohamed Asbahi, and Joel Yang, Institute of Materials and Research Engineering, Singapore

6:00-6:25 Modeling and Simulation for Solid-State Dewetting Problems *Weizhu Bao*, National University of Singapore, Singapore

6:30-6:55 Sharp-Interface Models for Solid-State Dewetting Problems Wei Jiang, Wuhan University, China

Wednesday, May 11

Mathematical Modeling of Microstructured Materials -Part II of IV

5:00 PM-7:00 PM

Room:Society Hill Ballroom A1

For Part 1 see MS111 For Part 3 see MS131

The goal of the minisymposium is to discuss the latest development in the area among mathematicians, material scientists and engineers, and identify important open problems. The list of topics includes but not limited to mathematical modeling of nanomaterials and biological nano-structures, homogenization and effective properties of composite materials, anisotropic behavior of composites with arbitrarily oriented inclusions and microcracks, analytical and numerical methods in periodic and random composites, inverse problems and microelectronic modeling.

Organizer: Lyudmyla Barannyk University of Idaho, USA

Organizer: Yuri Godin University of North Carolina, Charlotte, USA

Organizer: Yuliya Gorb University of Houston, USA

Organizer: Alexander Panchenko Washington State University, USA

5:00-5:25 Inverse Problems for the Schrödinger and Conductivity Problems on Networks

Fernando Guevara Vasquez, University of Utah, USA

MS121

Mathematical Modeling of Microstructured Materials -Part II of IV

5:00 PM-7:00 PM Room:Society Hill Ballroom A1 continued

5:30-5:55 Spectral Analysis and Computation of Effective Diffusivities for Steady Random Flows

N. Benjamin Murphy, Elena Cherkaev, and Jingyi Zhu, University of Utah, USA; Jack Xin, University of California, Irvine, USA; Kenneth M. Golden, University of Utah, USA

6:00-6:25 Fast Algorithm for Computing Effective Properties of Two-Phase Composites

Miao-Jung Y. Ou, University of Delaware, USA; Y.-H. Richard Tsai, University of Texas at Austin, USA; Wai-Yip Chan, Chinese University of Hong Kong, Hong Kong; Seong Jun Kim, Georgia Institute of Technology, USA

6:30-6:55 Soret Effects in Electrokinetically-Driven Heat Exchangers for Electronics Applications.

Silvia Jimenez Bolanos, Colgate University, USA; Burt S. Tilley and Bogdan M. Vernescu, Worcester Polytechnic Institute, USA

Wednesday, May 11

MS122

Numerical Methods for Low Reynolds Number Suspensions of Passive and Active Particles - Part I of II

5:00 PM-7:00 PM

Room:Society Hill Ballroom A2

For Part 2 see MS132

The dynamics of suspensions of rigid or flexible micron-scale particles that are either passive or active (self-propelled) is of great technological and biological interest. A number of numerical methods for modeling of periodic suspensions of Brownian spherical particles have been developed over the years; fewer methods exist capable of simulating suspensions of particles of more complex shapes in confined geometries. Of particular interest are methods that address active suspensions, the incorporation Brownian motion, and self-assembly. Focus will be on the development of mathematical and computational tools, but relevant scientific applications are also of interest.

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

5:00-5:25 Rigid Multiblob Models of Suspensions of Rigid Particles of Complex Shapes in Confinement

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

5:30-5:55 Modeling the Effect of Hydrophobicity on Nanoparticle Suspensions

Nikolaos Voulgarakis, Washington State University, USA

6:00-6:25 Immersed Particle Dynamics in Fluctuating Fluids with Memory

Christel Hohenegger, University of Utah, USA; Scott McKinley, University of Florida, USA

6:30-6:55 Frictional Interactions in Viscous Suspensions: Discontinuous Shear Thickening and Shear Jamming

Jeffrey Morris, City College of New York, USA

Wednesday, May 11

MS123 Variational Methods for Rods and Shells - Part I of III

5:00 PM-7:00 PM

Room:Cook

For Part 2 see MS133

Slender-body theories, such as rod and shell theories, are important for modelling materials such as biomembranes, graphene, nanotubes, semiconductor films, and smart fabrics. This minisymposium brings together researchers working on the wrinkling, delamination, confinement, and motion of slender elastic bodies, and on the rigorous derivation of slenderbody theories from three-dimensional nonlinear elasticity. The purpose of this minisymposium is also to exchange new tools in applied analysis and the calculus of variations, to allow us to face the mathematical challenges in developing the materials of tomorrow.

Organizer: David P. Bourne Durham University, United Kingdom

Organizer: Patrick Dondl Albert-Ludwigs-Universitat Freiburg, Germany

5:00-5:25 Large Motions of Nonlinearly Viscoelastic Rods and Shells

Stuart S. Antman, University of Maryland, College Park, USA; Alexey Stepanov, University of Maryland, USA; Suleyman Ulusoy, Zirve University, Turkey

5:30-5:55 A Model For Dislocations In Epitaxially Strained Elastic Films

Giovanni Leoni, Carnegie Mellon University, USA

6:00-6:25 On a Variational Model for the Elasticity of Biomembranes

Luca Lussardi, Università Cattolica del Sacro Cuore, Italy

6:30-6:55 Island Formation in Epitaxially Strained Films

Barbara Zwicknagl, University of Bonn, Germany
Wednesday, May 11

MS124

Soft Elastic Materials: Nonlinear Constitutive Models, Mathematical and Mechanical Aspects -Part III of III

5:00 PM-6:00 PM

Room:Flower

For Part 2 see MS114

Soft materials like rubber of soft biological tissues are subject to large elastic deformations. Anisotropy and other nonlinear effects in such materials leads to complex nonlinear models. The objective of the Minisymposium is to provide an overview of up-to-date research in the field and foster further interdisciplinary collaborations, through the consideration of both mechanical and mathematical aspects. The following topics will be addressed: - Advances in theoretical approaches - Symmetry analysis of BVPs in nonlinear elasticity - Exact solutions - Numerical aspects - Formulation and identification of constitutive models - Wave propagation aspects - Applications to soft biological tissues (arteries, biomembranes) -Stability issues

Organizer: Alexei F. Cheviakov University of Saskatchewan, Canada

Organizer: Jean-François Ganghoffer *LEMTA, Université de Lorraine, France*

5:00-5:25 Isotropic-Nematic Phase Transitions in Elastic Rigid Rod Newtorks

Carlos A. Garavito Garzon and Carme Calderer, University of Minnesota, USA

5:30-5:55 Fractional Modeling of Viscoelasticity in Cerebral Arteries and Aneurysms

Yue Yu, Lehigh University, USA; Paris Perdikaris, Massachusetts Institute of Technology, USA; George Em Karniadakis, Brown University, USA

Wednesday, May 11

MS125

Non-Equilibrium Phenomena for Liquid Crystals: Mathematical Case Studies - Part II of IV

5:00 PM-6:30 PM

Room:Bromley

For Part 1 see MS115 For Part 3 see MS135

Liquid crystals (LCs) are partially ordered materials. The mathematics of LCs for example, the Landau-de Gennes theory, raises challenging problems across the calculus of variations, partial differential equations, geometry and numerical analysis. This minisymposium is dedicated to non- equilibrium phenomena for LCs, in a non-variational setting that abound in applications such as nematic microfluidics, active matter and bio-materials. The talks address fundamental questions such as existence and regularity of solutions, effects of curvature and multiscale LC dynamics. A large proportion of the invited speakers are from under- represented research groups in the Far East, who have made recent contributions to the field.

Organizer: Changyou Wang Purdue University, USA

Organizer: Apala Majumdar University of Bath, United Kingdom

Organizer: Pingwen Zhang Peking University, China

5:00-5:25 Defect Behaviors of Liquid Crystals on a Spherical Surface: A Self-consistent Field Theory Simulation

Qin Liang, Xiangtan University, China

5:30-5:55 On the Local Controllability of Nematic Liquid Crystal Flow *Yuning Liu*, New York University-

Shanghai, China

6:00-6:25 Front Propagation for Nematic Liquid Crystals

Apala Majumdar, University of Bath, United Kingdom

Wednesday, May 11

MS126

Mechanics, Electro- and Hydro- dynamics of Drops and Vesicles - Part III of III

5:00 PM-7:00 PM

Room:Claypoole

For Part 2 see MS116

Drops and vesicles (self-enclosing unilamellar lipid bilayer) are ubiquitous in material sciences as their mechanics and dynamics are relevant to a wide range of engineering applications. Vesicles are used as biomimetic model membranes to shed light on how cell membranes uptake nano-particles and remodel under forces. The electrohydrodynamics of particles on the drop surface is investigated to understand how charged macromolecules transport on membranes. This minisymposium brings together experts in different aspects of this field to discuss new discoveries and novel mathematics for modeling the complex mechanics and dynamics of drops and vesicles as they interact with particles, charges and fluid in the context of biological soft materials.

Organizer: Yuan-Nan Young New Jersey Institute of Technology, USA

5:00-5:25 Deformation-Relaxation of Vesicles

Miao Yu, Rutgers University, USA; Rafael Lira, Max Planck Institute of Colloids and Interfaces, Germany; Karin Riske, Universidade Federal de São Paulo, Brazil; Rumiana Dimova, Max Planck Institute of Colloids and Interfaces, Germany; Hao Lin, Rutgers University, USA

5:30-5:55 Fluctuation and Dynamics of a Lipid Bilayer Membrane Under an Electric Field

Yuan-Nan Young, New Jersey Institute of Technology, USA; M.J. Miksis, Northwestern University, USA Wednesday, May 11

MS126

Mechanics, Electro- and Hydro- dynamics of Drops and Vesicles - Part III of III

5:00 PM-7:00 PM

Room:Claypoole continued

6:00-6:25 Multiscale Modeling of Mechanosensing Channels on Vesicles and Cell Membranes in 3D Constricted **Flows and Shear Flows**

Zhangli Peng, University of Notre Dame, USA; On Shun Pak, Santa Clara University, USA; Yuan-Nan Young, New Jersey Institute of Technology, USA

6:30-6:55 Complex Viscoelasticity of Shape Changes and Surface Hydrodynamics of Membrane **Protrusions**

Mohammad Rahimi, Princeton University, USA; Marino Arroyo, Universitat Politecnica de Catalunya, Spain; Margarita Staykova, Durham University, United Kingdom; Howard A. Stone, Princeton University, USA

Thursday, May 12

Registration 7:30 AM-3:30 PM Room:Society Hill Ballroom Foyer

Remarks 8:00 AM-8:15 AM Room:Society Hill Ballroom B,C,D,E

IP11 Issues in the Multiscale Modeling and Methods of Solids

8:15 AM-9:00 AM

Room:Society Hill Ballroom B,C,D,E

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

Pingbing Ming Chinese Academy of Sciences, China

Thursday, May 12

IP12

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

9:00 AM-9:45 AM

Room:Society Hill Ballroom B,C,D,E

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

Erica Lilleodden Helmholtz Zentrum Geesthacht, Germany

Coffee Break 9:45 AM-10:15 AM

Room: Hamilton Room





74

MS127

Mathematical and Computational Issues in Electromagnetic Materials -Part IV of V

10:15 AM-11:45 PM

Room:Society Hill Ballroom B

For Part 3 see MS117 For Part 5 see MS137

The aim of this minisymposium is to bring together researchers working on fundamental questions related to electromagnetic waves and materials and to highlight recent progress in this area. Topics of focus in this minisymposium include slow light, band gap solitons, photonics, metamaterials, and resonance.

Organizer: Aaron T. Welters Florida Institute of Technology, USA

Organizer: Robert P. Lipton Louisiana State University, USA

Organizer: Stephen P. Shipman Louisiana State University, USA

Organizer: Aaron T. Welters Florida Institute of Technology, USA

10:15-10:40 Mechanism of Absorption Suppression in Gyroscopic Systems Composed of High-Loss and Lossless Components

Alexander Figotin, University of California, Irvine, USA; Aaron T. Welters, Florida Institute of Technology, USA

10:45-11:10 Effective Properties of Periodic Tubular Structures

Yuri Godin, University of North Carolina, Charlotte, USA

11:15-11:40 Electric Quadrupolarizability of a Source-Driven Dielectric Sphere

Arthur D. Yaghjian, Electromagnetics Research Consultant, USA Thursday, May 12

MS128

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part VI of VII

10:15 AM-12:15 PM

Room:Society Hill Ballroom C

For Part 5 see MS118 For Part 7 see MS138

Colloidal nematic liquid crystals arise in a host of new applications including electrophoresis, microfluidic and display devices. Chromonic liquid crystals offer new perspectives and modeling tools in biology, e.g., in studies of DNA encapsulation. Both areas add new perspectives and challenges across liquid crystal research, including newly observed defect structures and novel liquid crystal flow problems. This minisymposium will focus on understanding of defects, flows with charged particles, mechanical properties of encapsulated anisotropic systems, as well as other related problems. The minisymposium will bring together physicists, mathematicians, and biologists who will discuss their recent work encompassing experiments, modeling, and analysis.

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Maria-Carme Calderer

University of Minnesota, USA

Organizer: Oleg Lavrentovich Kent State University, USA

10:15-10:40 A Finite Element Method for Nematic Liquid Crystals with Variable Degree of Orientation

Ricardo Nochetto, University of Maryland, College Park, USA; Shawn W. Walker, Louisiana State University, USA; Wujun Zhang, University of Maryland, USA

10:45-11:10 Numerical Approximation of the Ericksen Leslie Equations

Noel J. Walkington, Carnegie Mellon University, USA

11:15-11:40 Computational Modeling of Tactoid Dynamics in Chromonic Liquid Crystals

Chiqun Zhang, Noel J. Walkington, and Amit Acharya, Carnegie Mellon University, USA; Oleg Lavrentovich, Kent State University, USA

11:45-12:10 Exotic New Phases in Confined Chiral Liquid Crystals

Juan Hernandez-Ortiz, Universidad Nacional de Colombia, Colombia

MS129

Multiscale Modelling and Simulations of Dislocations for Continuum Plasticity-Part II of III

10:15 AM-12:15 PM

Room:Society Hill Ballroom D

For Part 1 see MS119 For Part 3 see MS139

This minisymposium is aimed to provide a platform for exchanging ideas over recent progress made in theoretical or computational considerations of dislocations on a multiscale basis. Attentions will be paid especially to the understanding of the connection between dislocation behaviour and continuum plasticity.

Organizer: Katrin Schulz Karlsruhe Institute of Technology, Germany

Organizer: Yichao Zhu Hong Kong University of Science and Technology, Hong Kong

10:15-10:40 Accounting for the Effect of Dislocations in Continuum Plasticity by Means of a Non-Local Spectral Formulation

Ricardo Lebensohn, Los Alamos National Laboratory, USA; Alan Needleman, Texas A&M University, USA

10:45-11:10 Homogenization of Dislocation Interactions in Regions of High Stress Concentrations

Katrin Schulz, Karlsruhe Institute of Technology, Germany

11:15-11:40 Modeling the Annealing of Thin Films on Lattice-Mismatched Substrates with Discrete Dislocation Dynamics

James J. Ramsey, U.S. Army Research Laboratory, USA

11:45-12:10 An A/C Study for Nano-Indentation and Homogeneous Dislocation Nucleation

Lei Zhang, Shanghai Jiao Tong University, China Thursday, May 12

MS130

Wetting/Dewetting in Complex Fluids and Thin Solid Films - Part III of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom E

For Part 2 see MS120 For Part 4 see MS140

Tremendous progress has been achieved in recent years on wetting/ dewetting problems in complex fluids and thin solid films, such as complex wetting phenomena on liquids, solidstate dewetting of thin films and moving contact lines dynamics. This minisymposium aims to promote interdisciplinary research collaborations among applied and computational mathematicians, and material scientists. Active experts and research groups in this field will deliver their thoughts and experiences on topics of wetting/dewetting from applied and computational mathematics, theoretical and experimental materials sciences, and discuss recent developments. possible collaborations and exciting future directions in the field of wetting/ dewetting.

Organizer: Weizhu Bao National University of Singapore, Singapore

Organizer: Wei Jiang Wuhan University, China

10:15-10:40 The Dynamics of Three-Phase Triple Junction and Contact Line *Xiaoping Wang*, Hong Kong University of Science and Technology, Hong Kong

10:45-11:10 Modeling and Simulation of Moving Contact Lines in Multi-Phase Fluids

Weiqing Ren, National University of Singapore and IHPC, Singapore

11:15-11:40 Modified Wenzel and Cassie Equations for Wetting on Rough Surfaces

Xianmin Xu, Chinese Academy of Sciences, China; Xiaoping Wang, Hong Kong University of Science and Technology, Hong Kong

11:45-12:10 Modeling and Simulation of Moving Contact Line Problem for Two-Phase Complex Fluids Flow

Zhen Zhang, South University of Science and Technology of China, China; Weiqing Ren, National University of Singapore and IHPC, Singapore

MS131 Mathematical Modeling of Microstructured Materials -Part III of IV

10:15 AM-12:15 PM

Room:Society Hill Ballroom A1

For Part 2 see MS121 For Part 4 see MS141

The goal of the minisymposium is to discuss the latest development in the area among mathematicians, material scientists and engineers, and identify important open problems. The list of topics includes but not limited to mathematical modeling of nanomaterials and biological nano-structures, homogenization and effective properties of composite materials, anisotropic behavior of composites with arbitrarily oriented inclusions and microcracks, analytical and numerical methods in periodic and random composites, inverse problems and microelectronic modeling.

Organizer: Lyudmyla Barannyk University of Idaho, USA

Organizer: Yuri Godin University of North Carolina, Charlotte, USA

Organizer: Yuliya Gorb University of Houston, USA

Organizer: Alexander Panchenko Washington State University, USA

10:15-10:40 Exact Relations and Links for Fiber-Reinforced Elastic Composites *Yury Grabovsky*, Temple University, USA

10:45-11:10 Discrete Breathers in a Resonant Granular Chain

Lifeng Liu, University of Pittsburgh, USA; Guillaume James, Inria Grenoble, France; Panayotis Kevrekidis, University of Massachusetts, USA; *Anna Vainchtein*, University of Pittsburgh, USA

11:15-11:40 Optimal Structures of Three-Dimensional Composites

Andrej V. Cherkaev, University of Utah, USA

11:45-12:10 Mesoscopic Modeling of Active Suspensions

Alexander Panchenko, Washington State University, USA

Thursday, May 12

MS132

Numerical Methods for Low Reynolds Number Suspensions of Passive and Active Particles - Part II of II

10:15 AM-11:45 AM

Room:Society Hill Ballroom A2

For Part 1 see MS122

The dynamics of suspensions of rigid or flexible micron-scale particles that are either passive or active (self-propelled) is of great technological and biological interest. A number of numerical methods for modeling of periodic suspensions of Brownian spherical particles have been developed over the years; fewer methods exist capable of simulating suspensions of particles of more complex shapes in confined geometries. Of particular interest are methods that address active suspensions, the incorporation Brownian motion, and self-assembly. Focus will be on the development of mathematical and computational tools, but relevant scientific applications are also of interest.

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

10:15-10:40 Transition to Collective Motion and Mixing in Suspensions of Micro-Rotors

Enkeleida Lushi, Brown University, USA

10:45-11:10 Understanding Particle Diffusion in Active Suspensions: A Multiscale Study

Blaise Delmotte, Courant Institute of Mathematical Sciences, New York University, USA

11:15-11:40 Stochastic Model of Clogging in a Microfluidic Device for Sorting Flexible Cells

Thomas Fai, Harvard University, USA

Thursday, May 12

MS133

Variational Methods for Rods and Shells - Part II of III

10:15 AM-12:15 PM

Room:Cook

For Part 1 see MS123 For Part 3 see MS142

Slender-body theories, such as rod and shell theories, are important for modelling materials such as biomembranes, graphene, nanotubes, semiconductor films, and smart fabrics. This minisymposium brings together researchers working on the wrinkling, delamination, confinement, and motion of slender elastic bodies, and on the rigorous derivation of slenderbody theories from three-dimensional nonlinear elasticity. The purpose of this minisymposium is also to exchange new tools in applied analysis and the calculus of variations, to allow us to face the mathematical challenges in developing the materials of tomorrow.

Organizer: David P. Bourne Durham University, United Kingdom

Organizer: Patrick Dondl Albert-Ludwigs-Universitat Freiburg, Germany

10:15-10:40 The Intrinsic Bending and Twisting of a Rod with Misfit

Robert V. Kohn and Ethan O'Brien, Courant Institute of Mathematical Sciences, New York University, USA

10:45-11:10 Nonlinear Bending Theories for Intrinsically Strained Plates

Peter Hornung, Technische Universität Dresden, Germany

11:15-11:40 Plates with Incompatible Strains

Marta Lewicka, University of Pittsburgh, USA

11:45-12:10 Interpenetration of Matter in Plate Theories Obtained as Gamma-Limits

Heiner Olbermann, University of Bonn, Germany; Eris Runa, Max Planck Institute for Mathematics in the Sciences, Germany

MS134

Materials Science Applications to Cellular and Molecular Structures -Part I of II

10:15 AM-11:45 AM

Room:Flower

For Part 2 see MS143

In the last decades, it has become clear that the genome is much more than the ATCG's that made up the DNA molecule, yet much remains unknown about its behavior in living cells. The genome is far from being a static information warehouse. Rather, it is a mechanically active entity that is constantly altering its shape. Since DNA molecules are in fact very long polymer molecules, a wealth of information can be gained about the behavior of the genome by applying principles from polymer theory. This minisymposium focuses on applications of polymer science to the studies of cellular organization and function.

Organizer: Erik Palmer University of South Carolina, USA

Organizer: Paula A. Vasquez University of South Carolina, USA

10:15-10:40 Polymeric Aspects of DNA Repair

Paula A. Vasquez, University of South Carolina, USA; Kerry Bloom, University of North Carolina, USA; M. Gregory Forest and Josh Lawrimore, University of North Carolina at Chapel Hill, USA

10:45-11:10 ChromoShake: A Chromosome Dynamics Simulator

Josh Lawrimore, Joseph Aicher, Patrick Hahn, Alyona Fulp, and Ben Kompa, University of North Carolina at Chapel Hill, USA; Leandra Vicci, University of North Carolina, USA; Michael Falvo and Russell M. Taylor II, University of North Carolina at Chapel Hill, USA; Kerry Bloom, University of North Carolina, USA

11:15-11:40 Cell-Ecm Interactions During Cancer Invasion

Yi Jiang, Georgia State University, USA

Thursday, May 12

MS135

Non-Equilibrium Phenomena for Liquid Crystals: Mathematical Case Studies -Part III of IV

10:15 AM-11:45 AM

Room:Bromley

For Part 2 see MS125 For Part 4 see MS144

Liquid crystals (LCs) are partially ordered materials. The mathematics of LCs for example, the Landau-de Gennes theory, raises challenging problems across the calculus of variations, partial differential equations, geometry and numerical analysis. This minisymposium is dedicated to non- equilibrium phenomena for LCs, in a non-variational setting that abound in applications such as nematic microfluidics, active matter and bio-materials. The talks address fundamental questions such as existence and regularity of solutions, effects of curvature and multiscale LC dynamics. A large proportion of the invited speakers are from under- represented research groups in the Far East, who have made recent contributions to the field.

Organizer: Changyou Wang Purdue University, USA

Organizer: Apala Majumdar University of Bath, United Kingdom

Organizer: Pingwen Zhang Peking University, China

10:15-10:40 Singular Limit Problem for Smectic Liquid Crystals

Jinhae Park, Chungnam National University, South Korea

10:45-11:10 Title Not Available

Margarida M. Telo Da Gama, University of Lisbon, Portugal

11:15-11:40 Global Existence and Regularity of Solutions for the Active Liquid Crystal System

Gui-Qiang Chen, University of Oxford, United Kingdom; Apala Majumdar, University of Bath, United Kingdom; *Dehua Wang* and Rongfang Zhang, University of Pittsburgh, USA

Thursday, May 12

MS136

On Limiting Strain Behaviour of Elastic Materials -Part I of II

10:15 AM-12:15 PM

Room:Claypoole

For Part 2 see MS145

In classical elasticity theory, there cannot be a nonlinear relationship between the linearized strain and the stress, which, in fact, is observed in some experiments. In this minisymposium we are interested in investigating the behaviour of elastic solids that are best described by implicit constitutive relations allowing for approximations where the linearized strain is a nonlinear function of the stress. This class of implicit constitutive models, developed by Rajagopal, are called strain-limiting models and their advantage is that they allow for the linearized strain to be bounded in all circumstances, even when the stress is very large.

Organizer: Yasemin Sengul Ozyegin University, Turkey

10:15-10:40 On Implicit and Strain-Limiting Theories for Describing the Elastic Response of Bodies

K. R. Rajagopal, Texas A&M University, USA

10:45-11:10 Limiting Strain Models in Elasticity Theory and Variational Integrals with Linear Growth

Miroslav Bulicek, Charles University in Prague, Czech Republic

11:15-11:40 On a Family of Inhomogeneous Torsional Creep Problems

Marian Bocea, Loyola University of Chicago, USA

11:45-12:10 Finitely Extensible Polymer Chains in Nematic Elastomers

Jamie M. Taylor, University of Oxford, United Kingdom

Lunch Break 12:15 PM-1:30 PM Attendees on their own

IP13 Can you Print your Toughness?

1:30 PM-2:15 PM

Room:Society Hill Ballroom B,C,D,E

Recent advances in material synthesis enable us to control material microstructure with unprecedented detail. This talk explores whether this ability can be exploited to create materials with unprecedented properties. Of particular interest are phenomena like fracture, dislocation dynamics, phase boundary propagation and peeling that are governed by the evolution of a free boundary or free discontinuity. In these phenomena, the effective behavior is not characterized by averaging, but instead dominated by critical events. Thus, the effective behavior can be qualitatively different from the local behavior. However, their characterization also raises difficult, but interesting, mathematical questions. This talk will explore these issues with selected examples.

Kaushik Bhattacharya California Institute of Technology, USA

Coffee Break 2:15 PM-2:45 PM Room:Hamilton Room



Thursday, May 12

MS137

Mathematical and Computational Issues in Electromagnetic Materials -Part V of V

2:45 PM-4:15 PM

Room:Society Hill Ballroom B

For Part 4 see MS127

The aim of this minisymposium is to bring together researchers working on fundamental questions related to electromagnetic waves and materials and to highlight recent progress in this area. Topics of focus in this minisymposium include slow light, band gap solitons, photonics, metamaterials, and resonance.

Organizer: Aaron T. Welters Florida Institute of Technology, USA

Organizer: Robert P. Lipton Louisiana State University, USA

Organizer: Stephen P. Shipman

Louisiana State University, USA

Organizer: Aaron T. Welters Florida Institute of Technology, USA

2:45-3:10 Nonlinear Models of Lasers, Noise, and the Salt Equations Steven Johnson, Massachusetts Institute of Technology, USA

3:15-3:40 Time-reversal Symmetry Bounds for Electromagnetic Devices *Andrea Au* and Dimitrios Sounas, The University of Texas at Austin, USA

3:45-4:10 Lossless Polariton Solitary Waves

Stephen P. Shipman, Louisiana State University, USA

Thursday, May 12

MS138

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part VII of VII

2:45 PM-4:45 PM

Room:Society Hill Ballroom C

For Part 6 see MS128

Colloidal nematic liquid crystals arise in a host of new applications including electrophoresis, microfluidic and display devices. Chromonic liquid crystals offer new perspectives and modeling tools in biology, e.g., in studies of DNA encapsulation. Both areas add new perspectives and challenges across liquid crystal research, including newly observed defect structures and novel liquid crystal flow problems. This minisymposium will focus on understanding of defects, flows with charged particles, mechanical properties of encapsulated anisotropic systems, as well as other related problems. The minisymposium will bring together physicists, mathematicians, and biologists who will discuss their recent work encompassing experiments, modeling, and analysis.

Organizer: Dmitry Golovaty University of Akron, USA

Organizer: Maria-Carme Calderer University of Minnesota, USA

Organizer: Oleg Lavrentovich Kent State University, USA

2:45-3:10 Electrokinetic Flows in Nematic Films with Prescribed Anchoring Patterns Oleh Tovkach, University of Akron, USA

MS138

Mathematical Problems in Nematic Colloids and Chromonic Liquid Crystals -Part VII of VII

2:45 PM-4:45 PM

Room:Society Hill Ballroom C

continued

3:15-3:40 Simulating Finite-Energy Disclination Dynamics by Modeling Discontinuous Director Fields

Chiqun Zhang, Carnegie Mellon University, USA; Xiaohan Zhang, Stanford University, USA; *Amit Acharya*, Carnegie Mellon University, USA; Dmitry Golovaty, University of Akron, USA; Noel J. Walkington, Carnegie Mellon University, USA

3:45-4:10 Orientation of a Liquid Crystal Layer with Arbitrary Anchoring Conditions

Eric P. Choate, Radford University, USA

4:15-4:40 Liquid Crystal Models of Viral Capsids

Javier Arsuaga, University of California, Davis, USA

Thursday, May 12

MS139

Multiscale Modelling and Simulations of Dislocations for Continuum Plasticity-Part III of III

2:45 PM-4:15 PM

Room:Society Hill Ballroom D

For Part 2 see MS129

This minisymposium is aimed to provide a platform for exchanging ideas over recent progress made in theoretical or computational considerations of dislocations on a multiscale basis. Attentions will be paid especially to the understanding of the connection between dislocation behaviour and continuum plasticity.

Organizer: Katrin Schulz Karlsruhe Institute of Technology, Germany

Organizer: Yichao Zhu Hong Kong University of Science and Technology, Hong Kong

2:45-3:10 Discrete Dislocation Dynamics with Anisotropic Elasticity Using Fast Fourier Transforms

Anthony Rollett, Carnegie Mellon University, USA; John Graham and Richard LeSar, Iowa State University, USA

3:15-3:40 Homogenisation of a Row of Dislocation Dipoles

Jon Chapman, University of Oxford, United Kingdom; Yang Xiang and *Yichao Zhu*, Hong Kong University of Science and Technology, Hong Kong

3:45-4:10 The Application of the String Method to the Dislocation Dynamics

Congming Jin, Zhejiang Sci-Tech University, China; Yang Xiang, Hong Kong University of Science and Technology, Hong Kong; Weiqing Ren, National University of Singapore and IHPC, Singapore; Gang Lu, California State University, Northridge, USA

Thursday, May 12

MS140

Wetting/Dewetting in Complex Fluids and Thin Solid Films - Part IV of IV

2:45 PM-4:15 PM

Room:Society Hill Ballroom E

For Part 3 see MS130

Tremendous progress has been achieved in recent years on wetting/ dewetting problems in complex fluids and thin solid films, such as complex wetting phenomena on liquids, solidstate dewetting of thin films and moving contact lines dynamics. This minisymposium aims to promote interdisciplinary research collaborations among applied and computational mathematicians, and material scientists. Active experts and research groups in this field will deliver their thoughts and experiences on topics of wetting/ dewetting from applied and computational mathematics, theoretical and experimental materials sciences, and discuss recent developments, possible collaborations and exciting future directions in the field of wetting/dewetting.

Organizer: Weizhu Bao

National University of Singapore, Singapore

Organizer: Wei Jiang Wuhan University, China

2:45-3:10 A Phase Field Approach for Simulating Solid-State Dewetting of Thin Films

Rachel Zucker, University of California, Berkeley, USA; Rainer Backofen and Axel Voigt, Technische Universität Dresden, Germany; W. Craig Carter and Carl V. Thompson, Massachusetts Institute of Technology, USA

3:15-3:40 Numerical Study of Vapor Condensation and Wetting Transition on Patterned Surface Using String Method

Yunzhi Li, National University of Singapore, Singapore

3:45-4:10 A Parametric Finite Element Method for Simulating Solid-State Dewetting Problems

Quan Zhao, National University of Singapore, Singapore

MS141

Mathematical Modeling of Microstructured Materials -Part IV of IV

2:45 PM-4:45 PM

Room:Society Hill Ballroom A1

For Part 3 see MS131

The goal of the minisymposium is to discuss the latest development in the area among mathematicians, material scientists and engineers, and identify important open problems. The list of topics includes but not limited to mathematical modeling of nanomaterials and biological nanostructures, homogenization and effective properties of composite materials, anisotropic behavior of composites with arbitrarily oriented inclusions and microcracks, analytical and numerical methods in periodic and random composites, inverse problems and microelectronic modeling.

Organizer: Lyudmyla Barannyk University of Idaho, USA

Organizer: Yuri Godin University of North Carolina, Charlotte, USA

Organizer: Yuliya Gorb University of Houston, USA

Organizer: Alexander Panchenko Washington State University, USA

2:45-3:10 Physically Motivated Model for Creep of Microstructured Materials to Study the Composite Effects at High Temperatures

Jürgen Albiez, Ioannis Sprenger, Anke Scherf, Martin Heilmaier, and Thomas Böhlke, Karlsruhe Institute of Technology, Germany

3:15-3:40 Fast Numerical Calculation of Percolation and Effective Diffusivity of Random Continuum Microstructures

Thomas J. Hardin and Christopher A. Schuh, Massachusetts Institute of Technology, USA

3:45-4:10 Network Representations of Mechanical Percolation

Sam B. Heroy, University of North Carolina at Chapel Hill, USA; Dane Taylor, University of Colorado Boulder, USA; Bill Shi, University of Chicago, USA; Peter J. Mucha, University of North Carolina, USA; Greg Forest, University of North Carolina at Chapel Hill, USA

4:15-4:40 The Morphology of Lath Martensite: A New Perspective

Anton Muehlemann, University of Oxford, United Kingdom; Konstantinos Koumatos, Gran Sasso Science Institute, Italy

Thursday, May 12

MS142

Variational Methods for Rods and Shells - Part III of III

2:45 PM-4:45 PM

Room:Cook

For Part 2 see MS133

Slender-body theories, such as rod and shell theories, are important for modelling materials such as biomembranes, graphene, nanotubes, semiconductor films, and smart fabrics. This minisymposium brings together researchers working on the wrinkling, delamination, confinement, and motion of slender elastic bodies, and on the rigorous derivation of slender-body theories from three-dimensional nonlinear elasticity. The purpose of this minisymposium is also to exchange new tools in applied analysis and the calculus of variations, to allow us to face the mathematical challenges in developing the materials of tomorrow.

Organizer: David P. Bourne Durham University, United Kingdom

Organizer: Patrick Dondl Albert-Ludwigs-Universitat Freiburg, Germany

2:45-3:10 A Bending Theory for Nematic Elastomers

Paul Plucinsky and Kaushik Bhattacharya, California Institute of Technology, USA

3:15-3:40 Elastic Curves and Surfaces in Riemannian Spaces with Applications to Interpolation of Shells

P.-A. Absil and Gousenbourger Pierre-Yves, Université Catholique de Louvain, Belgium; Paul Striewski and *Benedikt Wirth*, Universität Münster, Germany

MS142

Variational Methods for Rods and Shells - Part III of III

2:45 PM-4:45 PM

Room:Cook

continued

3:45-4:10 Geodesic Calculus for Smooth and Discrete Shells

Behrend Heeren and Martin Rumpf, University of Bonn, Germany; Peter Schroeder, California Institute of Technology, USA; Max Wardetzky, University of Göttingen, Germany; Benedikt Wirth, Universität Münster, Germany

4:15-4:40 Phase Field Models with Topological Constraints

Stephan Wojtowytsch, Durham University, United Kingdom Thursday, May 12

MS143

Materials Science Applications to Cellular and Molecular Structures -Part II of II

2:45 PM-4:15 PM

Room:Flower

For Part 1 see MS134

In the last decades, it has become clear that the genome is much more than the ATCG's that made up the DNA molecule, yet much remains unknown about its behavior in living cells. The genome is far from being a static information warehouse. Rather, it is a mechanically active entity that is constantly altering its shape. Since DNA molecules are in fact very long polymer molecules, a wealth of information can be gained about the behavior of the genome by applying principles from polymer theory. This minisymposium focuses on applications of polymer science to the studies of cellular organization and function.

Organizer: Erik Palmer University of South Carolina, USA

Organizer: Paula A. Vasquez University of South Carolina, USA

2:45-3:10 Mathematical Insight in Biofilm Structure and Function

Jia Zhao, University of South Carolina, USA

3:15-3:40 Numerical Approximation of Non-Newtonian Fluid Structure Interaction Problems

Hyesuk Lee, Clemson University, USA

3:45-4:10 A Three-Dimensional Elastic Model for Hydrogel Mechanics *Hao Chen*, Georgia State University,

USA

Thursday, May 12

MS144

Non-Equilibrium Phenomena for Liquid Crystals: Mathematical Case Studies - Part IV of IV

2:45 PM-4:15 PM

Room:Bromley

For Part 3 see MS135

Liquid crystals (LCs) are partially ordered materials. The mathematics of LCs for example, the Landau-de Gennes theory, raises challenging problems across the calculus of variations, partial differential equations, geometry and numerical analysis. This minisymposium is dedicated to non- equilibrium phenomena for LCs, in a non-variational setting that abound in applications such as nematic microfluidics, active matter and bio-materials. The talks address fundamental questions such as existence and regularity of solutions, effects of curvature and multiscale LC dynamics. A large proportion of the invited speakers are from under- represented research groups in the Far East, who have made recent contributions to the field.

Organizer: Changyou Wang Purdue University, USA

Organizer: Apala Majumdar University of Bath, United Kingdom

Organizer: Pingwen Zhang Peking University, China

2:45-3:10 Tensor Model for Bent-Core Molecules Based on Molecular Theory *Jie Xu*, Peking University, China

3:15-3:40 Liquid-Crystalline Behavior and Elastic Properties of Homopolymer Interfaces Containing Rod-Coil Diblock Copolymers *Pingwen Zhang*, Peking University, China

3:45-4:10 Decoupled, Energy Stable Scheme for Continuum Hydrodynamics Allen-Cahn and Cahn-Hilliard Phase Field Model Hui Zhang, Beijing Normal University, China

MS145 On Limiting Strain Behaviour of Elastic Materials -

Part II of II

2:45 PM-4:15 PM

Room:Claypoole

For Part 1 see MS136

In classical elasticity theory, there cannot be a nonlinear relationship between the linearized strain and the stress, which, in fact, is observed in some experiments. In this minisymposium we are interested in investigating the behaviour of elastic solids that are best described by implicit constitutive relations allowing for approximations where the linearized strain is a nonlinear function of the stress. This class of implicit constitutive models, developed by Rajagopal, are called strainlimiting models and their advantage is that they allow for the linearized strain to be bounded in all circumstances, even when the stress is very large.

Organizer: Yasemin Sengul Ozyegin University, Turkey

2:45-3:10 Implicit Theories for Fluids

Giuseppe Saccomandi, Università di Perugia, Italy

3:15-3:40 On Hyperelasticity and Rank--1 Convexity for Strain--limiting Theories of Elasticity

Jay R. Walton, Texas A&M University, USA

3:45-4:10 Traveling Waves in One-Dimensional Nonlinear Models of Strain-Limiting Viscoelasticity

Yasemin Sengul, Ozyegin University, Turkey

Notes

Abstracts



Mathematical Aspects of Materials Science

Abstracts are printed as submitted by the authors.

Notes

Speaker and Organizer Index



Mathematical Aspects of Materials Science

Α

A.H. Shehadeh, Hala, MS43, 10:15 Mon A.H. Shehadeh, Hala, MS43, 10:45 Mon A.H. Shehadeh, Hala, MS54, 2:30 Mon A.H. Shehadeh, Hala, MS65, 5:00 Mon Abeynanda, Gayan S., PP1, 8:00 Mon Acharya, Amit, MS119, 5:00 Wed Acharya, Amit, MS138, 3:15 Thu Ackerman, David, MS75, 11:45 Tue Aharoni, Hillel, MS2, 11:45 Sun Aharoni, Hillel, MS104, 11:45 Wed Ahn, Surl-Hee, MS10, 10:15 Sun Al Mosleh, Salem H., MS13, 4:00 Sun Alaimo, Francesco, MS49, 4:00 Mon Alali, Bacim, MS51, 2:30 Mon Alali, Bacim, MS62, 5:00 Mon Alali, Bacim, MS73, 10:15 Tue Alali, Bacim, MS83, 2:30 Tue Alali, Bacim, MS83, 2:30 Tue Alali, Bacim, MS93, 5:00 Tue Alama, Stan, MS98, 10:45 Wed Albiez, Jürgen, MS141, 2:45 Thu Albin, Nathan, MS62, 6:00 Mon Alix-Williams, Darius, PP1, 8:00 Mon Alu, Andrea, MS87, 5:00 Tue Antman, Stuart S., MS123, 5:00 Wed Aqua, Jean-Noel, MS70, 11:15 Tue Aristoff, David, MS75, 10:15 Tue Aristoff, David, MS85, 2:30 Tue Aronson, Igor S., MS49, 2:30 Mon Aronson, Igor S., MS52, 2:30 Mon Aroyo, Mois I., MS23, 5:00 Sun Arroyave, Ray, MS95, 5:00 Tue Arsuaga, Javier, MS138, 4:15 Thu Asta, Mark, MS3, 10:45 Sun Atherton, Timothy J., MS7, 10:15 Sun Atherton, Timothy J., MS18, 2:30 Sun Atherton, Timothy J., MS29, 5:00 Sun Atherton, Timothy J., MS29, 5:00 Sun Atherton, Timothy J., MS40, 10:15 Mon Au, Andrea, MS137, 3:15 Thu

В

Ball, John, MS108, 2:30 Wed
Banerjee, Amartya S., MS15, 3:30 Sun
Bao, Weizhu, MS99, 10:15 Wed
Bao, Weizhu, MS110, 2:30 Wed
Bao, Weizhu, MS120, 5:00 Wed
Bao, Weizhu, MS120, 6:00 Wed
Bao, Weizhu, MS130, 10:15 Thu
Bao, Weizhu, MS140, 2:45 Thu
Barajas-Solano, David A., MS84, 3:00 Tue

Barannyk, Lyudmyla, MS93, 5:30 Tue Barannyk, Lyudmyla, MS111, 2:30 Wed Barannyk, Lyudmyla, MS121, 5:00 Wed Barannyk, Lyudmyla, MS131, 10:15 Thu Barannyk, Lyudmyla, MS141, 2:45 Thu Bardsley, Patrick, MS91, 5:00 Tue Barmak, Katayun, MS25, 5:00 Sun Barrales-Mora, Luis, MS14, 3:30 Sun Baskaran, Arvind, MS43, 11:15 Mon Baskaran, Arvind, MS68, 11:45 Tue Bauman, Patricia, MS118, 6:00 Wed Beach, Geoffrey, MS55, 2:30 Mon Begau, Christoph, MS119, 6:30 Wed Beller, Daniel, MS88, 6:00 Tue Bellis, Cedric, MS71, 11:15 Tue Berdichevsky, Victor, MS111, 3:00 Wed Berezovski, Mihhail, MS87, 6:30 Tue Beris, Antony N., PP1, 8:00 Mon Bernacki, Marc, MS14, 4:00 Sun Bernstein, Noam, MS39, 11:45 Mon Bevan, Jonathan J., MS114, 3:30 Wed Bhattacharya, Kaushik, IP13, 1:30 Thu Bian, X, MS74, 10:15 Tue Bian, Xin, MS74, 10:15 Tue Bian, Xin, MS84, 2:30 Tue Bian, Xin, MS94, 5:00 Tue Birnir, Bjorn, MS46, 2:30 Mon Biskup, Marek, MS11, 10:15 Sun Blum, Volker, MS26, 5:00 Sun Bluman, George, MS104, 10:15 Wed

Bocea, Marian, MS136, 11:15 Thu Boechler, Nicholas, MS96, 5:30 Tue Boffi, Nicholas M., PP1, 8:00 Mon Bonnet-Ben Dhia, Anne Sophie, MS56, 5:00 Mon

Bonnetier, Eric, MS45, 2:30 Mon Booty, Michael R., MS116, 3:30 Wed Borcea, Ciprian S., MS1, 10:15 Sun Borg, Matthew K., MS74, 11:45 Tue Bou-Rabee, Nawaf, MS85, 2:30 Tue Bourne, David P., MS24, 5:00 Sun Bourne, David P., MS123, 5:00 Wed Bourne, David P., MS133, 10:15 Thu Bourne, David P., MS142, 2:45 Thu Bouzid, Mehdi, PP1, 8:00 Mon Bradley, R. Mark, MS80, 3:00 Tue Braun, Benjamin, MS55, 3:00 Mon Braun, Julian, MS72, 10:15 Tue Bronsard, Lia, MS88, 5:00 Tue Bulatov, Vasily, IP3, 1:30 Sun Bulicek, Miroslav, MS136, 10:45 Thu Burke, Christopher J., MS18, 4:00 Sun

С

Calderer, Maria-Carme, MS78, 2:30 Tue Calderer, Maria-Carme, MS88, 5:00 Tue Calderer, Maria-Carme, MS98, 10:15 Wed Calderer, Maria-Carme, MS108, 2:30 Wed Calderer, Maria-Carme, MS118, 5:00 Wed Calderer, Maria-Carme, MS118, 5:00 Wed Calderer, Maria-Carme, MS128, 10:15 Thu Calderer, Maria-Carme, MS138, 2:45 Thu Cances, Eric, MS4, 10:15 Sun Cances, Eric, MS48, 2:30 Mon Cances, Eric, MS59, 5:00 Mon Canevari, Giacomo, MS108, 4:00 Wed Capella Kort, Antonio, MS66, 6:00 Mon

Cassier, Maxence, MS5, 10:15 Sun Cassier, Maxence, MS16, 2:30 Sun Cassier, Maxence, MS16, 2:30 Sun Cassier, Maxence, MS27, 5:00 Sun Cassier, Maxence, MS38, 10:15 Mon Cassier. Maxence. MS71. 10:15 Tue Cassier, Maxence, MS81, 2:30 Tue Cassier, Maxence, MS91, 5:00 Tue Cassier, Maxence, MS91, 6:00 Tue Cassier, Maxence, MS101, 10:15 Wed Ceniceros, Hector D., MS17, 2:30 Sun Chattoraj, Joyjit, MS40, 11:45 Mon Chen, Bryan G., MS67, 11:45 Tue Chen, Hao, MS143, 3:45 Thu Chen, Huajie, MS37, 10:45 Mon Chen, Xian, MS69, 11:15 Tue Cherednichenko, Kirill, MS33, 5:00 Sun Cherkaev, Andrej V., MS131, 11:15 Thu Cherkaev, Elena, MS27, 5:30 Sun Cherkaev, Elena, MS62, 5:00 Mon Cherkaev, Elena, MS81, 3:30 Tue Cherkos, Alemayehu, PP1, 8:00 Mon Cheviakov, Alexei F., MS104, 10:15 Wed Cheviakov, Alexei F., MS104, 10:45 Wed Cheviakov, Alexei F., MS114, 2:30 Wed Cheviakov, Alexei F., MS124, 5:00 Wed Chirikjian, Gregory, MS34, 10:45 Mon Choate, Eric P., MS138, 3:45 Thu Choi, Minseok, MS74, 11:15 Tue Clemmer, Joel T., MS7, 11:45 Sun Collins, Lincoln, MS91, 6:30 Tue Comer, Jeffrey, MS85, 4:00 Tue Constantin, Costel, MS65, 5:30 Mon Cook, L. Pamela, MS73, 10:15 Tue Copic, Martin, MS88, 6:30 Tue Costa, Timothy, MS83, 3:00 Tue Cromer, Michael, MS8, 10:15 Sun Cromer, Michael, MS8, 10:15 Sun Cromer, Michael, MS19, 2:30 Sun Cromer, Michael, MS30, 5:00 Sun Crone, Joshua C., MS119, 6:00 Wed

Csányi, Gábor, IP6, 8:15 Tue Cui, Colin, MS10, 11:45 Sun Cuitino, Alberto, MS20, 4:00 Sun

D Dahmen, Karin, MS18, 2:30 Sun Dai, Shibin, MS113, 4:00 Wed Dai, Shuyang, MS99, 10:45 Wed Damle, Anil, MS4, 11:45 Sun Das, Shuvrangsu, PP1, 8:00 Mon Dassbach, Paula, PP1, 8:00 Mon Davidovitch, Benny, MS13, 2:30 Sun Davtyan, Aram, MS31, 6:00 Sun Dayal, Kaushik, MS31, 5:00 Sun Dayal, Kaushik, MS82, 2:30 Tue de las Penas, Ma. Louise N., MS1, 10:45 Sun Debenedictis, Andrew, PP1, 8:00 Mon Del Gado, Emanuela, MS19, 2:30 Sun D'Elia, Marta, MS17, 4:00 Sun Delmotte, Blaise, MS132, 10:45 Thu Di Fratta, Giovanni, MS44, 11:45 Mon Diehl, Patrick, MS93, 6:00 Tue Dirr, Nicolas, MS22, 2:30 Sun Dobson, Matthew, MS85, 4:30 Tue Dondl, Patrick, MS123, 5:00 Wed Dondl, Patrick, MS133, 10:15 Thu Dondl, Patrick, MS142, 2:45 Thu Donev, Aleksandar, MS122, 5:00 Wed Doney, Aleksandar, MS122, 5:00 Wed Donev, Aleksandar, MS132, 10:15 Thu Donovan, Preston, PP1, 8:00 Mon Du, Qiang, MS103, 11:45 Wed

Ε

E, Weinan, MS46, 3:00 Mon Earls, Ashley, PP1, 8:00 Mon Ehrlacher, Virginie, MS28, 5:30 Sun Elbanna, Ahmed, MS40, 10:15 Mon El-Borai, Mahmoud M., PP1, 8:00 Mon Elder, Ken, MS64, 5:30 Mon Elder, Ken, MS68, 10:45 Tue Emelianenko, Maria, MS3, 10:15 Sun Emelianenko, Maria, MS14, 2:30 Sun Emelianenko, Maria, MS25, 5:00 Sun Emelianenko, Maria, MS36, 10:15 Mon Emelianenko, Maria, MS47, 2:30 Mon Emelianenko, Maria, MS53, 3:30 Mon Emelianenko, Maria, MS58, 5:00 Mon Emelianenko, Maria, MS95, 5:00 Tue Emelianenko, Maria, MS105, 10:15 Wed Engel, Michael, MS9, 11:15 Sun Eon, Jean-Guillaume, MS1, 10:15 Sun Eon, Jean-Guillaume, MS12, 2:30 Sun Eon, Jean-Guillaume, MS23, 5:00 Sun Eon, Jean-Guillaume, MS34, 10:15 Mon Epshteyn, Yekaterina, MS36, 10:45 Mon Esedoglu, Selim, MS3, 10:15 Sun Esedoglu, Selim, MS6, 10:15 Sun Esedoglu, Selim, MS14, 2:30 Sun Esedoglu, Selim, MS25, 5:00 Sun Esedoglu, Selim, MS36, 10:15 Mon Esedoglu, Selim, MS47, 2:30 Mon Esedoglu, Selim, MS58, 5:00 Mon Esedoglu, Selim, MS68, 10:15 Tue Espanol, Malena I., MS43, 10:15 Mon Espanol, Malena I., MS54, 2:30 Mon Espanol, Malena I., MS54, 2:30 Mon Espanol, Malena I., MS65, 5:00 Mon Evans, Davis, PP1, 8:00 Mon Evans, James, MS9, 10:15 Sun Evans, James, MS42, 10:45 Mon Evans, James, MS57, 6:00 Mon Evans, Jim W., MS9, 10:15 Sun Evans, Jim W., MS20, 2:30 Sun Evans, Jim W., MS31, 5:00 Sun

F

Fai, Thomas, MS132, 11:15 Thu Falk, Michael L., MS7, 10:15 Sun Falk, Michael L., MS7, 10:45 Sun Falk, Michael L., MS18, 2:30 Sun Falk, Michael L., MS29, 5:00 Sun Falk, Michael L., MS40, 10:15 Mon Farmer, Brittan A., MS54, 3:00 Mon Fattebert, Jean-Luc, PP1, 8:00 Mon Fichthorn, Kristen, MS9, 10:45 Sun Figotin, Alexander, MS127, 10:15 Thu Fischer, Julian, MS80, 4:00 Tue Foiles, S. M., MS3, 11:15 Sun Foldes, Robert, PP1, 8:00 Mon Fonseca, Irene, MS103, 10:15 Wed Forest, M. Gregory, MS30, 5:00 Sun Forest, M. Gregory, MS41, 10:15 Mon Forest, M. Gregory, MS41, 10:45 Mon Forest, M. Gregory, MS52, 2:30 Mon Forest, M. Gregory, MS63, 5:00 Mon Friesecke, Gero, MS4, 10:15 Sun Friesecke, Gero, MS15, 2:30 Sun Friesecke, Gero, MS26, 5:00 Sun Friesecke, Gero, MS37, 10:15 Mon Fu, Szu-Pei, MS116, 4:00 Wed Fukushima, Ryoki, MS11, 11:15 Sun Furer, Joshua, PP1, 8:00 Mon

G

Ganghoffer, Jean-François, MS104, 10:15 Wed Ganghoffer, Jean-François, MS104, 11:15 Wed Ganghoffer, Jean-François, MS114, 2:30 Wed Ganghoffer, Jean-François, MS124, 5:00 Wed Gao, Weiguo, MS109, 2:30 Wed Garavito Garzon, Carlos A., MS124, 5:00 Wed Garcia Cervera, Carlos, MS6, 10:15 Sun Garcia Cervera, Carlos, MS17, 2:30 Sun Garcia Cervera, Carlos, MS28, 5:00 Sun Garcia-Cervera, Carlos, MS44, 10:45 Mon Garcia-Cervera, Carlos, MS75, 11:15 Tue Garikipati, Krishna, MS40, 11:15 Mon Garroni, Adriana, MS72, 10:45 Tue Gavini, Vikram, MS26, 6:00 Sun Gemmer, John A., MS35, 11:15 Mon

Genovese, Luigi, MS26, 5:30 Sun Gibou, Frederic G., MS42, 10:15 Mon Gibou, Frederic G., MS53, 2:30 Mon Gibou, Frederic G., MS53, 2:30 Mon Gibou, Frederic G., MS64, 5:00 Mon Gill, Simon, MS90, 6:00 Tue Giomi, Luca, MS60, 5:00 Mon Giorgi, Tiziana, MS108, 3:00 Wed Glicksman, Martin E., MS47, 3:00 Mon Godin, Yuri, MS111, 2:30 Wed Godin, Yuri, MS111, 4:00 Wed Godin, Yuri, MS121, 5:00 Wed Godin, Yuri, MS131, 10:15 Thu Godin, Yuri, MS127, 10:45 Thu Godin, Yuri, MS141, 2:45 Thu Golden, Kenneth, MS16, 3:00 Sun Golden, Kenneth M., MS81, 2:30 Tue Golovaty, Dmitry, MS3, 10:15 Sun Golovaty, Dmitry, MS14, 2:30 Sun Golovaty, Dmitry, MS25, 5:00 Sun Golovaty, Dmitry, MS36, 10:15 Mon Golovaty, Dmitry, MS47, 2:30 Mon Golovaty, Dmitry, MS58, 5:00 Mon Golovaty, Dmitry, MS78, 2:30 Tue Golovaty, Dmitry, MS88, 5:00 Tue Golovaty, Dmitry, MS98, 10:15 Wed Golovaty, Dmitry, MS108, 2:30 Wed Golovaty, Dmitry, MS108, 3:30 Wed Golovaty, Dmitry, MS118, 5:00 Wed Golovaty, Dmitry, MS128, 10:15 Thu Golovaty, Dmitry, MS138, 2:45 Thu Golubovic, Leonardo, MS70, 10:45 Tue Gorb, Yuliya, MS111, 2:30 Wed Gorb, Yuliya, MS121, 5:00 Wed Gorb, Yuliya, MS131, 10:15 Thu Gorb, Yuliya, MS141, 2:45 Thu Grabovsky, Yury, MS131, 10:15 Thu Grason, Gregory M., MS35, 11:45 Mon Griffiths, Ian, MS115, 2:30 Wed Grimm, Uwe, MS34, 11:15 Mon Griva, Igor, MS95, 5:00 Tue Griva, Igor, MS95, 6:30 Tue

Griva, Igor, MS105, 10:15 Wed Gu, Yejun, MS89, 5:30 Tue Guenneau, Sebastien, MS77, 3:00 Tue Guevara Vasquez, Fernando, MS71, 10:15 Tue Guevara Vasquez, Fernando, MS81, 2:30 Tue Guevara Vasquez, Fernando, MS91, 5:00 Tue Guevara Vasquez, Fernando, MS101, 10:15 Wed Guevara Vasquez, Fernando, MS121, 5:00 Wed Gustafsson, Mats, MS16, 3:30 Sun Gygi, Francois, MS15, 2:30 Sun н

Haataja, Mikko, IP2, 9:00 Sun Han, Yilong, MS109, 3:00 Wed Hardin, Thomas J., MS141, 3:15 Thu Harmandaris, Vagelis, MS39, 10:15 Mon Harmandaris, Vagelis, MS39, 10:45 Mon Harmandaris, Vagelis, MS50, 2:30 Mon Harmandaris, Vagelis, MS61, 5:00 Mon Harmon, Michael D., PP1, 8:00 Mon Harrison, Matt P., MS90, 6:30 Tue Harutyunyan, Davit, MS35, 10:15 Mon Hashmi, Javeria, PP1, 8:00 Mon Hawkins, Rhoda, MS49, 3:30 Mon Heeren, Behrend, MS142, 3:45 Thu Heitzinger, Clemens, MS75, 10:45 Tue Henao, Duvan, MS24, 5:30 Sun Henao, Duvan, MS98, 11:45 Wed Hernandez, Efrain, MS21, 4:00 Sun Hernandez-Ortiz, Juan, MS128, 11:45 Thu Heroy, Sam B., MS141, 3:45 Thu

Herrmann, Michael, MS86, 3:00 Tue Hiltner, Lindsey, PP1, 8:00 Mon Hinkle, Adam R., PP1, 8:00 Mon Hochrainer, Thomas, MS82, 3:30 Tue Hochrainer, Thomas, MS119, 5:30 Wed Hoffman, Aaron, MS86, 3:30 Tue Hohenegger, Christel, MS122, 6:00 Wed Holm, Elizabeth, MS14, 2:30 Sun Holmes-Cerfon, Miranda, MS12, 3:00 Sun Hornung, Peter, MS133, 10:45 Thu

Hu, Jilong, MS115, 4:00 Wed Hu, Xiangyu, MS112, 3:00 Wed Huang, Tao, MS115, 3:00 Wed Hubenthal, Mark, MS101, 10:15 Wed Hurley, Ryan C., MS18, 3:00 Sun

J

Jabin, Pierre-Emmanuel, MS113, 2:30 Wed James, Guillaume, MS86, 2:30 Tue Jedrasiak, Patryk, PP1, 8:00 Mon Jensen, Katharine E., MS18, 3:30 Sun Jiang, Jiahua, PP1, 8:00 Mon Jiang, Shidong, MS89, 6:00 Tue Jiang, Wei, MS110, 2:30 Wed Jiang, Wei, MS120, 5:00 Wed Jiang, Wei, MS120, 6:30 Wed Jiang, Wei, MS130, 10:15 Thu Jiang, Wei, MS140, 2:45 Thu Jiang, Yi, MS134, 11:15 Thu Jimenez Bolanos, Silvia, MS51, 2:30 Mon Jimenez Bolanos, Silvia, MS62, 5:00 Mon Jimenez Bolanos, Silvia, MS73, 10:15 Tue Jimenez Bolanos, Silvia, MS83, 2:30 Tue Jimenez Bolanos, Silvia, MS93, 5:00 Tue Jimenez Bolanos, Silvia, MS121, 6:30 Wed Jin, Congming, MS139, 3:45 Thu Johnson, Steven, MS137, 2:45 Thu Jonoska, Natasha, MS12, 2:30 Sun Joo, Sookyung, MS78, 3:30 Tue

K Kamien, Randall, MS78, 2:30 Tue Kang, Hyeonbae, MS56, 6:00 Mon Katsoulakis, Markos A., MS20, 2:30 Sun

Kattner, Ursula, MS95, 5:30 Tue Kaxiras, Efthimios, MS48, 2:30 Mon Kent, Andrew, MS44, 10:15 Mon Kevrekidis, Panayotis, MS96, 6:00 Tue Kfoury, Ralph, MS106, 11:15 Wed *Khenner, Mikhail V., MS70, 10:15 Tue Khenner, Mikhail V., MS80, 2:30 Tue Khenner, Mikhail V., MS80, 2:30 Tue Khenner, Mikhail V., MS90, 5:00 Tue Khenner, Mikhail V., MS100, 10:15 Wed*

Kinderlehrer, David, IP5, 9:00 Mon Knees, Dorothee, MS22, 3:00 Sun Knezevic, Marko, MS14, 3:00 Sun Kohn, Robert V., MS2, 10:15 Sun Kohn, Robert V., MS13, 2:30 Sun Kohn, Robert V., MS24, 5:00 Sun Kohn, Robert V., MS35, 10:15 Mon Kohn, Robert V., MS133, 10:15 Thu Kordy, Michal A., MS101, 10:45 Wed Koukkari, Pertti S., MS95, 6:00 Tue Kraczek, Brent, PP1, 8:00 Mon Kraft, Daniela J., MS115, 3:30 Wed Krajcevski, Mile, MS1, 10:15 Sun Krajcevski, Mile, MS12, 2:30 Sun Krajcevski, Mile, MS23, 5:00 Sun Krajcevski, Mile, MS34, 10:15 Mon Krill III, Carl E., IP4, 8:15 Mon Kupferman, Raz, MS29, 6:30 Sun

Lagarias, Jeffrey, MS23, 5:30 Sun Lai, Ru-Yu, MS71, 10:45 Tue Lamacz, Agnes, MS33, 5:30 Sun Laux, Tim, MS25, 6:30 Sun Lavrentovich, Maxim O., MS35, 10:45 Mon Lavrentovich, Oleg, MS78, 2:30 Tue Lavrentovich, Oleg, MS88, 5:00 Tue Lavrentovich, Oleg, MS98, 10:15 Wed Lavrentovich, Oleg, MS108, 2:30 Wed Lavrentovich, Oleg, MS118, 5:00 Wed Lavrentovich, Oleg, MS128, 10:15 Thu Lavrentovich, Oleg, MS138, 2:45 Thu Lawrimore, Josh, MS134, 10:45 Thu Lazar, Emanuel A., PP1, 8:00 Mon Lazar, Emanuel A., MS79, 4:00 Tue Lebensohn, Ricardo, MS129, 10:15 Thu Lee, Hyesuk, MS143, 3:15 Thu Lehoucq, Richard B., MS112, 2:30 Wed Lei, Huan, MS10, 10:15 Sun Lei, Huan, MS10, 10:45 Sun Lei, Huan, MS21, 2:30 Sun Lei, Huan, MS32, 5:00 Sun Leimkuhler, Ben, MS61, 5:00 Mon Leimkuhler, Benedict, MS39, 10:15 Mon Leimkuhler. Benedict. MS50. 2:30 Mon Leimkuhler, Benedict, MS61, 5:00 Mon Leiter, Kenneth, PP1, 8:00 Mon León Baldelli, Andrés A, MS24, 6:00 Sun Leoni, Giovanni, MS123, 5:30 Wed Lewicka, Marta, MS29, 5:30 Sun Lewicka, Marta, MS133, 11:15 Thu Li, Jing, MS10, 10:15 Sun Li, Jing, MS10, 11:15 Sun Li, Jing, MS21, 2:30 Sun Li, Jing, MS32, 5:00 Sun Li, Xiantao, MS6, 10:15 Sun Li, Xiantao, MS4, 11:15 Sun Li, Xiantao, MS17, 2:30 Sun Li, Xiantao, MS28, 5:00 Sun Li, Xingjie, MS21, 3:30 Sun Li, Xingjie, MS99, 11:15 Wed Li, Yunzhi, MS140, 3:15 Thu Li, Zhen, MS102, 11:45 Wed Liang, Qin, MS125, 5:00 Wed Lilleodden, Erica, IP12, 9:00 Thu Lin, Lin, MS4, 10:15 Sun Lin, Lin, MS6, 11:45 Sun Lin, Lin, MS15, 2:30 Sun Lin, Lin, MS26, 5:00 Sun Lin, Lin, MS37, 10:15 Mon

Lin, Lin, MS37, 11:45 Mon Lipton, Robert P., MS51, 2:30 Mon Lipton, Robert P., MS97, 10:15 Wed Lipton, Robert P., MS97, 10:15 Wed Lipton, Robert P., MS107, 2:30 Wed Lipton, Robert P., MS117, 5:00 Wed Lipton, Robert P., MS127, 10:15 Thu Lipton, Robert P., MS137, 2:45 Thu Liu, Andrea, MS7, 11:15 Sun Liu, Chun, MS41, 11:15 Mon Liu, Chun, MS73, 11:15 Tue Liu, Da-Jiang, MS20, 3:00 Sun Liu, Di, MS48, 3:30 Mon Liu, Liping, MS6, 11:15 Sun Liu, Yuning, MS125, 5:30 Wed liverpool, Tanniemola, MS52, 3:00 Mon Lowengrub, John, IP7, 9:00 Tue Lu, Jianfeng, MS4, 10:15 Sun Lu, Jianfeng, MS15, 2:30 Sun Lu, Jianfeng, MS17, 3:00 Sun Lu, Jianfeng, MS26, 5:00 Sun Lu, Jianfeng, MS37, 10:15 Mon Lu, Jianfeng, MS39, 11:15 Mon Lu, Jianfeng, MS79, 3:00 Tue Lu, Jianfeng, MS103, 10:15 Wed Lu, Jianfeng, MS113, 2:30 Wed Lund, Ross, MS66, 6:30 Mon Luo, Tao, MS79, 3:30 Tue Lushi, Enkeleida, MS132, 10:15 Thu Lussardi, Luca, MS123, 6:00 Wed

Μ

Ma, Xiao, PP1, 8:00 Mon Maday, Yvon, MS15, 3:00 Sun Mahadevan, L, MS2, 11:15 Sun *Majumdar, Apala, MS115, 2:30 Wed Majumdar, Apala, MS125, 5:00 Wed* Majumdar, Apala, MS125, 6:00 Wed *Majumdar, Apala, MS135, 10:15 Thu Majumdar, Apala, MS144, 2:45 Thu* Maksov, Artem, PP1, 8:00 Mon Mamonov, Alexander V., MS101, 11:15 Wed Manning, Lisa, MS40, 10:45 Mon Margetis, Dionisios, MS9, 10:15 Sun Margetis, Dionisios, MS20, 2:30 Sun Margetis, Dionisios, MS31, 5:00 Sun Margetis, Dionisios, MS42, 10:15 Mon Margetis, Dionisios, MS53, 2:30 Mon Margetis, Dionisios, MS64, 5:00 Mon Margetis, Dionisios, MS64, 5:00 Mon Margetis, Dionisios, MS103, 10:15 Wed Margetis, Dionisios, MS113, 2:30 Wed Maroudas, Dimitrios, MS80, 3:30 Tue Masnada, Elian, MS19, 4:00 Sun Mason, Daniel, MS89, 5:00 Tue Massoudi, Mehrdad, PP1, 8:00 Mon Matthews, Charles, MS50, 3:00 Mon McColm, Gregory, MS1, 10:15 Sun McColm, Gregory, MS12, 2:30 Sun McColm, Gregory, MS23, 5:00 Sun McColm, Gregory, MS34, 10:15 Mon Mchenry, Emily A., PP1, 8:00 Mon McPhedran, Ross, MS5, 10:45 Sun Melcher, Christof, MS55, 4:00 Mon Mengesha, Tadele, MS51, 3:30 Mon Menon, Govind, MS36, 11:15 Mon Mießen, Christian, MS89, 6:30 Tue Miksis, Michael, MS106, 10:15 Wed Militzer, Matthias, MS58, 5:30 Mon Miller, Owen D., MS38, 10:45 Mon Millien, Pierre, MS56, 5:30 Mon Milton, Graeme, MS5, 10:15 Sun Milton, Graeme W., MS5, 10:15 Sun Milton, Graeme W., MS16, 2:30 Sun Milton, Graeme W., MS27, 5:00 Sun Milton, Graeme W., MS38, 10:15 Mon Milton, Graeme W., MS71, 10:15 Tue Milton, Graeme W., MS67, 11:15 Tue Ming, Pingbing, IP11, 8:15 Thu Ming, Pingbing, MS6, 10:15 Sun Ming, Pingbing, MS17, 2:30 Sun Ming, Pingbing, MS28, 5:00 Sun Mitchell, John A., MS3, 11:45 Sun Mohammadi, Ali, PP1, 8:00 Mon

Montero, Alberto, MS98, 11:15 Wed Morris, Jeffrey, MS122, 6:30 Wed Moskow, Shari, MS81, 3:00 Tue Muehlemann, Anton, MS141, 4:15 Thu *Muratov, Cyrill B., MS44, 10:15 Mon Muratov, Cyrill B., MS55, 2:30 Mon Muratov, Cyrill B., MS66, 5:00 Mon* Murphy, N. Benjamin, MS121, 5:30 Wed Mwasame, Paul, MS30, 6:30 Sun

Ν

Needleman, Dan, MS63, 5:30 Mon Nepomnyashchy, Alexander, MS25, 5:30 Sun Nepomnyashchy, Alexander, MS70, 11:45 Tue Nespolo, Massimo, MS23, 6:00 Sun Neukamm, Stefan, MS11, 10:15 Sun Neukamm, Stefan, MS11, 10:45 Sun Neukamm, Stefan, MS22, 2:30 Sun Neukamm, Stefan, MS33, 5:00 Sun Neumann, Philipp, MS94, 6:00 Tue Nguyen, Dinh Liem, MS87, 5:30 Tue Nguven, Hoai-Minh, MS45, 2:30 Mon Nguyen, Hoai-Minh, MS56, 5:00 Mon Nguyen, Hoai-Minh, MS67, 10:15 Tue Nguyen, Hoai-Minh, MS77, 2:30 Tue Nguyen, Hoai-Minh, MS87, 5:00 Tue Nguyen, Hoai-Minh, MS101, 11:45 Wed Nguyen, Hoang Loc, MS91, 5:30 Tue Nguyen, Loc, MS45, 3:30 Mon Nie, Qin, MS41, 11:45 Mon Nigam, Nilima, MS117, 5:30 Wed Nochetto, Ricardo, MS128, 10:15 Thu Nolte, Florian, MS44, 11:15 Mon Novick-Cohen, Amy, MS25, 6:00 Sun Novick-Cohen, Amy, MS110, 3:30 Wed

Ola, Petri, MS45, 3:00 Mon Olbermann, Heiner, MS133,

Olbermann, Heiner, MS133, 11:45 Thu Olmsted, Peter, MS8, 11:15 Sun Olson, Derek, MS69, 11:45 Tue O'Neil, Michael, MS117, 6:00 Wed Onofrei, Daniel, MS77, 3:30 Tue Otis, Richard, MS105, 10:45 Wed Otto, Felix, IP1, 8:15 Sun *Ou, Miao-Jung Y., MS51, 2:30 Mon Ou, Miao-Jung Y., MS62, 5:00 Mon Ou, Miao-Jung Y., MS73, 10:15 Tue* Ou, Miao-Jung Y., MS73, 10:45 Tue *Ou, Miao-Jung Y., MS83, 2:30 Tue* Ou, Miao-Jung Y., MS121, 6:00 Wed *Ou, Miao-Jung Y., MS93, 5:00 Tue* Ou, Yvonne, MS38, 11:15 Mon

Ö Özer, Teoman, MS114, 2:30 Wed

Ρ

Palmer, Erik, MS30, 5:30 Sun Palmer, Erik, MS134, 10:15 Thu Palmer, Erik, MS143, 2:45 Thu Pan, W., MS84, 2:30 Tue Pan, Wenxiao, MS74, 10:15 Tue Pan, Wenxiao, MS84, 2:30 Tue Pan, Wenxiao, MS94, 5:00 Tue Pan, Wenxiao, MS102, 10:15 Wed Pan, Wenxiao, MS112, 2:30 Wed Pan, Wenxiao, MS112, 3:30 Wed Panagiotou, Eleni, MS8, 11:45 Sun Panchenko, Alexander, MS111, 2:30 Wed Panchenko, Alexander, MS121, 5:00 Wed Panchenko, Alexander, MS131, 10:15 Thu Panchenko, Alexander, MS131, 11:45 Thu Panchenko, Alexander, MS141, 2:45 Thu Pankov, Alexander, MS97, 11:15 Wed Park, Jinhae, MS135, 10:15 Thu Patrone, Paul, MS43, 10:15 Mon Pearson, Daniel A., MS100, 10:15 Wed Pego, Robert, MS46, 3:30 Mon Peletier, Mark, MS72, 10:15 Tue

Peletier, Mark, MS82, 2:30 Tue Peletier, Mark, MS92, 5:00 Tue Peletier, Mark, MS103, 10:45 Wed Peng, Zhangli, MS126, 6:00 Wed Perdikaris, Paris, MS84, 3:30 Tue Pham, Trung, PP1, 8:00 Mon Phillips, Daniel, MS78, 3:00 Tue Pick, Adi, PP1, 8:00 Mon Pierre-Louis, Oliver, MS53, 3:00 Mon Pierre-Louis, Oliver, MS90, 5:30 Tue Pierre-Louis, Oliver, MS110, 4:00 Wed Pierre-Louis, Olivier, PP1, 8:00 Mon Pikovsky, Arkady, MS76, 10:45 Tue Pinaud, Olivier, MS75, 10:15 Tue Pinaud, Olivier, MS85, 2:30 Tue Piro, Markus, MS105, 10:15 Wed Plechac, Petr, MS9, 10:15 Sun Plechac, Petr, MS20, 2:30 Sun Plechac, Petr, MS31, 5:00 Sun Plechac, Petr, MS68, 11:15 Tue Plucinsky, Paul, MS65, 6:00 Mon Plucinsky, Paul, MS142, 2:45 Thu Polizzi, Eric, MS75, 10:15 Tue Ponte Castaneda, Pedro, MS62, 5:30 Mon Potestio, Raffaello, MS94, 5:00 Tue Pradhan, Dr. Sahadev, MS47, 3:30 Mon Praprotnik, Matej, MS74, 10:45 Tue Pribram-Jones, Aurora, MS15, 4:00 Sun Prodan, Emil, MS4, 10:45 Sun

Prodan, Emil, MS5, 11:15 Sun Proserpio, Davide M., MS1, 11:15 Sun Purohit, Prashant K., MS76, 11:45 Tue Putinar, Mihai, MS5, 10:15 Sun Putinar, Mihai, MS16, 2:30 Sun Putinar, Mihai, MS27, 5:00 Sun Putinar, Mihai, MS38, 10:15 Mon Putinar, Mihai, MS38, 10:15 Mon

Quer, Jannes, MS50, 3:30 Mon

Q

R

Rabkin, Eugen, MS110, 3:00 Wed Radu, Petronela, MS93, 5:00 Tue Rahimi, Mohammad, MS126, 6:30 Wed Rajagopal, K. R., MS136, 10:15 Thu Ramaswamy, Rajesh, MS60, 6:00 Mon Ramsey, James J., MS129, 11:15 Thu Ratsch, Christian, MS42, 10:15 Mon Ratsch, Christian, MS42, 10:15 Mon Ratsch, Christian, MS53, 2:30 Mon Ratsch, Christian, MS64, 5:00 Mon Ratsch, Christian, MS57, 5:30 Mon Reina, Celia, MS82, 3:00 Tue Ren, Weiqing, MS6, 10:45 Sun Ren, Weiging, MS130, 10:45 Thu Ren, Xinguo, MS48, 3:00 Mon Renardy, Michael, MS8, 10:45 Sun Rey, Alejandro D., MS41, 10:15 Mon Rinderspacher, B. Chistopher, MS31, 6:30 Sun

Robbins, Jonathan, MS66, 5:30 Mon Rollett, Anthony, MS58, 6:00 Mon Rollett, Anthony, MS139, 2:45 Thu Ruan, Dihui, PP1, 8:00 Mon Rycroft, Chris H., MS7, 10:15 Sun

S

Saccomandi, Giuseppe, MS114, 3:00 Wed Saccomandi, Giuseppe, MS145, 2:45 Thu Salac, David, MS116, 3:00 Wed Salipante, Paul, MS106, 10:45 Wed Santangelo, Christian, MS2, 10:15 Sun Sbalzarini, Ivo F., MS60, 5:30 Mon Scardia, Lucia, MS72, 11:15 Tue Schäffner, Mathias, MS33, 6:00 Sun Schäffner, Mathias, PP1, 8:00 Mon Schlömerkemper, Anja, MS28, 5:00 Sun Schneider, Reinhold, MS37, 10:15 Mon Schöberl, Markus, MS21, 4:30 Sun Schotland, John, MS107, 3:30 Wed Schroeder, Joerg, MS92, 5:30 Tue

Schulte, Egon, MS34, 10:15 Mon Schulz, Katrin, MS119, 5:00 Wed Schulz, Katrin, MS129, 10:15 Thu Schulz, Katrin, MS129, 10:45 Thu Schulz, Katrin, MS139, 2:45 Thu Schulze, Tim. MS46, 2:30 Mon Schulze, Tim, MS57, 5:00 Mon Schulze, Tim, MS57, 5:00 Mon Schulze, Tim, MS68, 10:15 Tue Schulze, Tim, MS69, 10:45 Tue Schütte, Christof, IP10, 1:30 Wed Schweizer, Ben, MS77, 2:30 Tue Seleson, Pablo, MS43, 11:45 Mon Seleson, Pablo, MS51, 3:00 Mon Sen, Surajit, MS96, 5:00 Tue Senechal, Marjorie, MS1, 10:15 Sun Senechal, Marjorie, MS12, 2:30 Sun Senechal, Marjorie, MS23, 5:00 Sun Senechal, Marjorie, MS34, 10:15 Mon Sengul, Yasemin, MS136, 10:15 Thu Sengul, Yasemin, MS145, 2:45 Thu Sengul, Yasemin, MS145, 3:45 Thu Shang, Xiaocheng, MS39, 10:15 Mon Shang, Xiaocheng, MS50, 2:30 Mon Shang, Xiaocheng, MS61, 5:00 Mon Shang, Xiaocheng, MS61, 6:30 Mon Shankar, Varun, MS102, 11:15 Wed Shapeev, Alexander, MS92, 5:00 Tue Sharon, Eran, MS29, 6:00 Sun Shelley, Michael J., MS63, 5:00 Mon Shipman, Stephen P., MS137, 3:45 Thu Shipman, Stephen P., MS97, 10:15 Wed Shipman, Stephen P., MS107, 2:30 Wed Shipman, Stephen P., MS107, 2:30 Wed Shipman, Stephen P., MS117, 5:00 Wed Shipman, Stephen P., MS127, 10:15 Thu Shipman, Stephen P., MS137, 2:45 Thu Shirokoff, David, PP1, 8:00 Mon Silling, Stewart, MS102, 10:15 Wed Simpson, Gideon, MS85, 3:00 Tue Simpson, Gideon, MS107, 3:00 Wed Sinno, Talid, MS31, 5:30 Sun

Sjöberg, Daniel, MS27, 6:00 Sun Slastikov, Valery, MS44, 10:15 Mon Slastikov, Valery, MS55, 2:30 Mon Slastikov, Valery, MS66, 5:00 Mon Song, Dawei, PP1, 8:00 Mon Souvignier, Bernd, MS23, 6:30 Sun Spencer, Brian J., MS90, 5:00 Tue Srolovitz, David J., MS58, 5:00 Mon Srolovitz, David J., MS69, 10:15 Tue Srolovitz, David J., MS120, 5:00 Wed Stachura, Eric, MS45, 4:00 Mon Stachura, Eric, MS97, 11:45 Wed Starosvetsky, Yuli, MS76, 10:15 Tue Starosvetsky, Yuli, MS76, 11:15 Tue Starosvetsky, Yuli, MS86, 2:30 Tue Starosvetsky, Yuli, MS96, 5:00 Tue Stinis, Panos, MS21, 2:30 Sun Stoltz, Gabriel, MS50, 2:30 Mon Stoltz, Gabriel, MS59, 5:00 Mon Streinu, Ileana, MS1, 11:45 Sun Strubbe, David A., MS59, 5:30 Mon Stukowski, Alexander, MS54, 3:30 Mon Sukhinin, Alexey, MS107, 4:00 Wed Sullivan, Daniel, PP1, 8:00 Mon Sun, Jonathan, MS66, 5:00 Mon

T

Tadmor, Ellad B., MS39, 10:15 Mon Tang, Yu-Hang, MS112, 4:00 Wed Tao, Yunzhe, MS73, 11:45 Tue Taylor, Jamie M., MS136, 11:45 Thu Taylor, Jean, MS12, 3:30 Sun Teich, Erin G., MS12, 4:00 Sun Telo Da Gama, Margarida M., MS135, 10:45 Thu *Thaler, Andrew E., MS71, 10:15 Tue Thaler, Andrew E., MS81, 2:30 Tue* Thaler, Andrew E., MS81, 4:00 Tue *Thaler, Andrew E., MS91, 5:00 Tue Thaler, Andrew E., MS91, 5:00 Tue Thaler, Andrew E., MS101, 10:15 Wed Theil, Florian, MS72, 10:15 Tue Theil, Florian, MS82, 2:30 Tue*

Theil, Florian, MS92, 5:00 Tue Thomas, Spencer L., MS109, 3:30 Wed Thompson, Carl V., MS110, 2:30 Wed Tian, Xiaochuan, MS83, 3:30 Tue Tibballs, John E., PP1, 8:00 Mon Tobasco, Ian, MS2, 10:45 Sun Torquato, Salvatore, MS111, 3:30 Wed Torrejon, Diego, MS36, 11:45 Mon Tovkach, Oleh, MS138, 2:45 Thu Trask, Nathaniel, MS102, 10:15 Wed Trask, Nathaniel, MS102, 10:45 Wed Trask, Nathaniel, MS112, 2:30 Wed Tretiakov, Oleg, MS55, 3:30 Mon Triki, Faouzi, MS67, 10:45 Tue Trstanova, Zofia, MS61, 5:30 Mon Tsagkarogiannis, Dimitrios, MS61, 6:00 Mon Turc, Catalin, MS97, 10:45 Wed Twarock, Reidun, IP9, 9:00 Wed

U Urata, Shingo, MS28, 6:30 Sun

V Vainchtein, Anna, MS76, 10:15 Tue Vainchtein, Anna, MS76, 10:15 Tue Vainchtein, Anna, MS86, 2:30 Tue Vainchtein, Anna, MS96, 5:00 Tue Vainchtein, Anna, MS131, 10:45 Thu Van Koten, Brian, MS85, 3:30 Tue Vasquez, Paula A., MS134, 10:15 Thu Vasquez, Paula A., MS134, 10:15 Thu Vasquez, Paula A., MS143, 2:45 Thu Veerapaneni, Shravan, MS116, 2:30 Wed Vella, Dominic, MS13, 3:30 Sun Venkataramani, Shankar C., MS13, 3:00 Sun Venkatesh, Vishwas, PP1, 8:00 Mon Vinals, Jorge, MS118, 5:30 Wed Vinoles, Valentin, MS87, 6:00 Tue Vlachos, Dion, MS20, 3:30 Sun Voigt, Axel, MS42, 11:15 Mon Voigt, Axel, MS49, 2:30 Mon

Voigt, Axel, MS49, 3:00 Mon Voigt, Axel, MS60, 5:00 Mon Voigt, Axel, MS57, 6:30 Mon Voorhees, Peter, MS3, 10:15 Sun Voulgarakis, Nikolaos, MS122, 5:30 Wed

W

Wagner, Caroline, MS30, 6:00 Sun Walker, Shawn W., MS88, 5:30 Tue Walkington, Noel J., MS128, 10:45 Thu Walton, Jay R., MS145, 3:15 Thu Wan, Xiaoliang, MS21, 3:00 Sun Wang, Changyou, MS115, 2:30 Wed Wang, Changyou, MS125, 5:00 Wed Wang, Changyou, MS135, 10:15 Thu Wang, Changyou, MS144, 2:45 Thu Wang, Dehua, MS135, 11:15 Thu Wang, Lin-Wang, MS59, 6:00 Mon Wang, Qi, MS41, 10:15 Mon Wang, Qi, MS52, 2:30 Mon Wang, Qi, MS52, 3:30 Mon Wang, Qi, MS63, 5:00 Mon Wang, Xiaoping, IP8, 8:15 Wed Wang, Xiaoping, MS130, 10:15 Thu Wang, Xin Cindy, MS37, 11:15 Mon Warren, James, MS47, 2:30 Mon Watson, Stephen J., MS70, 10:15 Tue Watson, Stephen J., MS70, 10:15 Tue Watson, Stephen J., MS80, 2:30 Tue Watson, Stephen J., MS90, 5:00 Tue Watson, Stephen J., MS100, 10:15 Wed Waurick, Marcus, MS22, 3:30 Sun Weare, Jonathan, MS9, 11:45 Sun Wei, Chaozhen, MS100, 10:45 Wed Weinstein, Michael I., MS67, 10:15 Tue Wellander, Niklas, MS11, 11:45 Sun Welters, Aaron T., MS5, 10:15 Sun Welters, Aaron T., MS16, 2:30 Sun Welters, Aaron, MS27, 5:00 Sun Welters, Aaron T., MS27, 5:00 Sun Welters, Aaron, MS38, 10:15 Mon Welters, Aaron T., MS97, 10:15 Wed

Welters, Aaron T., MS107, 2:30 Wed Welters, Aaron T., MS117, 5:00 Wed Welters, Aaron T., MS117, 5:00 Wed Welters, Aaron T., MS127, 10:15 Thu Welters, Aaron T., MS137, 2:45 Thu Wilber, J. Patrick, MS65, 5:00 Mon Wilkinson, Mark, MS113, 3:00 Wed Wilkinson, Mark, MS118, 6:30 Wed Wirth, Benedikt, MS113, 3:30 Wed Wirth, Benedikt, MS142, 3:15 Thu Wojtowytsch, Stephan, MS142, 4:15 Thu

Wright, Doug, MS86, 4:00 Tue Wu, Xiaojie, MS28, 6:00 Sun Wynne, Patrick M., PP1, 8:00 Mon

Χ

Xiang, Yang, MS69, 10:15 Tue Xiang, Yang, MS79, 2:30 Tue Xiang, Yang, MS89, 5:00 Tue Xiang, Yang, MS99, 10:15 Wed Xiang, Yang, MS103, 11:15 Wed Xiang, Yang, MS109, 2:30 Wed Xu, Jie, MS144, 2:45 Thu Xu, Xianmin, MS130, 11:15 Thu

Y

Yaghjian, Arthur D., MS127, 11:15 Thu Yang, Chao, MS26, 6:30 Sun Yang, Chao, MS48, 2:30 Mon Yang, Chao, MS59, 5:00 Mon Yang, Jiang, MS51, 4:00 Mon Yang, Jinkyu, MS96, 6:30 Tue Yang, Xiu, MS10, 10:15 Sun Yang, Xiu, MS21, 2:30 Sun Yang, Xiu, MS32, 5:00 Sun Yang, Zhijian, MS6, 10:15 Sun Yang, Zhijian, MS17, 2:30 Sun Yang, Zhijian, MS28, 5:00 Sun Yasuda, Shugo, MS94, 5:30 Tue Yazdani, Alireza, MS84, 4:00 Tue Yi, Xin, MS106, 11:45 Wed Yip, Aaron, MS79, 2:30 Tue

Young, Yuan-Nan, MS106, 10:15 Wed Young, Yuan-Nan, MS116, 2:30 Wed Young, Yuan-Nan, MS126, 5:00 Wed Young, Yuan-Nan, MS126, 5:30 Wed Yu, Jianguo, PP1, 8:00 Mon Yu, Miao, MS126, 5:00 Wed Yu, Yue, MS124, 5:30 Wed

Ζ

Zahedi, Ramin, PP1, 8:00 Mon Zarnescu, Arghir, MS98, 10:15 Wed Zeiner, Peter, MS34, 11:45 Mon Zemlyanova, Anna, MS111, 2:30 Wed Zhang, Chiqun, MS128, 11:15 Thu Zhang, Hai, MS99, 11:45 Wed Zhang, Hui, MS63, 6:00 Mon Zhang, Hui, MS144, 3:45 Thu Zhang, Lei, MS17, 3:30 Sun Zhang, Lei, MS129, 11:45 Thu Zhang, Luchan, MS109, 4:00 Wed Zhang, Pingwen, MS115, 2:30 Wed Zhang, Pingwen, MS125, 5:00 Wed Zhang, Pingwen, MS135, 10:15 Thu Zhang, Pingwen, MS144, 2:45 Thu Zhang, Pingwen, MS144, 3:15 Thu Zhang, Wei, MS50, 4:00 Mon Zhang, Xuewei, PP1, 8:00 Mon Zhang, Yong-Wei, MS120, 5:30 Wed Zhang, Zhen, MS130, 11:45 Thu Zhao, Jia, MS41, 10:15 Mon Zhao, Jia, MS52, 2:30 Mon Zhao, Jia, MS52, 4:00 Mon Zhao, Jia, MS63, 5:00 Mon Zhao, Jia, MS143, 2:45 Thu Zhao, Quan, MS140, 3:45 Thu Zhou, Lin, MS8, 10:15 Sun Zhou, Lin, MS19, 2:30 Sun Zhou, Lin, MS19, 3:30 Sun Zhou, Lin, MS30, 5:00 Sun Zhou, Zhi, MS83, 4:00 Tue Zhu, Yichao, MS119, 5:00 Wed Zhu, Yichao, MS129, 10:15 Thu

Zhu, Yichao, MS139, 2:45 Thu Zhu, Yichao, MS139, 3:15 Thu Zoellner, Dana, MS3, 10:15 Sun Zoellner, Dana, MS14, 2:30 Sun Zoellner, Dana, MS25, 5:00 Sun Zoellner, Dana, MS36, 10:15 Mon Zoellner, Dana, MS36, 10:15 Mon Zoellner, Dana, MS47, 2:30 Mon Zoellner, Dana, MS58, 5:00 Mon Zou, Weizhong, MS19, 3:00 Sun Zucker, Rachel, MS140, 2:45 Thu Žumer, Slobodan, MS78, 4:00 Tue Zwicknagl, Barbara, MS123, 6:30 Wed Zyskin, Maxim, PP1, 8:00 Mon

MS16 Budget

Conference Budget SIAM Conference on Mathematical Aspects of Materials Science May 8-12, 2016 Philadelphia, PA Expected Paid Attendance 450

Expected Faid Attendance		400	
Revenue			
Registration Income		\$164,655	
	Total	\$164,655	
Expenses			
Printing		\$4,084.00	
Organizing Committee		\$3,000.00	
Invited Speakers		\$15,800.00	
Food and Beverage		\$19,194.00	
AV Equipment and Telecommunication		\$18,500.00	
Advertising		\$3,700.00	
Conference Labor (including benefits)		\$40,952.00	
Other (supplies, staff travel, freight, misc.)		\$5,759.00	
Administrative		\$10,643.00	
Accounting/Distribution & Shipping		\$5,710.00	
Information Systems		\$10,584.00	
Customer Service		\$3,853.00	
Office Space (Building)		\$0,019.00 \$2,014.00	
Other SIAM Services		\$3,914.00	
	Total	\$155,692	
Net Conference Revenue		\$8,963	
Estimated Support for Travel Awards not included above:			

14 \$10,985
14

Sheraton Philadelphia Society Hill Hotel

