Final Program

SIAM Conference on Computational Science and Engineering

February 27-March 3, 2017
Hilton Atlanta, Atlanta, Georgia, USA

Sponsored by the SIAM Activity Group on
Computational Science and Engineering (CSE)

The SIAM Activity Group on Computational Science and Engineering (CSE) fosters collaboration and interaction among applied mathematicians, computer scientists, domain scientists and engineers in those areas of research related to the theory, development, and use of computational technologies for the solution of important problems in science and engineering. The activity group promotes computational science and engineering as an academic discipline and promotes simulation as a mode of scientific discovery on the same level as theory and experiment.

The activity group organizes the biennial SIAM Conference on Computational Science and Engineering and maintains a wiki, a membership directory, and an electronic mailing list. The SIAG recently established the SIAG/CSE Early Career Prize.

A new status report, Research and Education in Computational Science and Engineering, is available as a preprint from the SIAG CSE Wiki or directly from *https://arxiv.org/abs/1610.02608*. The article summarizes the status of CSE as an emerging discipline and presents the trends and challenges for the field.

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Scan the QR code with any QR reader and download the TripBuilder EventMobile™ app to your iPhone, iPad, iTouch or Android mobile device. You can also visit *www.tripbuildermedia.com/apps/siam2017*

Society for Industrial and Applied Mathematics
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SIAM Registration Desk

The SIAM registration desk is located in the 1st floor foyer. It is open during the following hours:

Sunday, February 26
1:00 PM - 8:00 PM

Monday, February 27
7:45 AM - 5:00 PM

Tuesday, February 28
7:00 AM - 5:00 PM

Wednesday, March 1
7:30 AM - 5:00 PM

Thursday, March 2
7:45 AM - 5:00 PM

Friday, March 3
7:45 AM - 12:00 PM

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Atlanta, GA 30303, USA
Direct Telephone: +1-404-659-2000
Toll Free Reservations (USA and Canada): 1-800-HILTONS
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Hotel Telephone Number

To reach an attendee or leave a message, call +1-404-659-2000. If the attendee is a hotel guest, the hotel operator can connect you with the attendee's room.

Hotel Check-in and Check-out Times

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

Child Care

The Hilton Atlanta recommends TLC Sitters of Atlanta (*http://www.tlcsittersofatlanta.com/*) 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, non-member attendees who are employed by the following organizations are entitled to the SIAM member registration rate.

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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 January 2017.

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 for their support of this conference.

Join SIAM and save!

Leading the applied mathematics community . . .

SIAM members save up to $130 on full registration for the 2017 SIAM Conference on Computational Science and Engineering (CSE17)! 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 Computational Science and Engineering (SIAG/CSE). As a SIAG/CSE 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/CSE 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:

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E-mail: membership@siam.org

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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

Attendees booked within the SIAM room block will receive complimentary wireless Internet access in their guest rooms. Complimentary wireless Internet access in the meeting space is also available to SIAM attendees.

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/CSE members)
Coffee breaks daily
Room set-ups and audio/visual equipment
Poster Sessions
Welcome Reception

Job Postings

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

Poster Blitzes and Plenary Poster Sessions including Minisymposteria

There are two plenary poster sessions featuring Minisymposteria. Minisymposteria are collections of three or more posters by different presenters grouped around a central theme.

Poster sessions will take place in the Galleria on both Tuesday, Feburary 28 and Wednesday, March 1 from 4:30 PM – 6:30 PM. Both sessions include Minisymposteria and general posters grouped by category. Poster Blitzes will precede each poster session at 3:10 PM in Ballroom D - 2nd Fl.

To ensure conference participants have ample time to view posters, presenters are requested to keep their posters on display for two full days, from 8:00 AM on Tuesday, February 28 through 6:30 PM on Wednesday, March 1. Presenters are expected to stand by their posters during their assigned session.

Posters will be reviewed for poster prizes! These sessions provide a great opportunity to network and are a great prelude to dinner in Atlanta!

Important Notice to Electronic Poster Presenters

Poster Session 1, PP1: Electronic Posters, is scheduled on Tuesday, February 28, 4:30 – 6:30 PM in the Galleria Room. Presenters may use their own computers to connect to the electronic display or they may use the computers provided by connecting a pre-loaded flash drive. Electronic poster presenters may begin setup of their displays at 3:00 PM on Tuesday, February 28.

Important Notice to General Poster Presenters

Plenary poster sessions are scheduled on Tuesday, February 28, 4:30 – 6:30 PM and Wednesday, March 1, 4:30 – 6:30 PM.

General Poster Presenters may set up beginning 6:00 PM on Sunday, February 26. All materials must be posted by 8:00 AM on Tuesday, February 28. To ensure conference participants have ample time to view posters, presenters are requested to keep their posters on display for two full days, from 8:00 AM on Tuesday, February 28 through 6:30 PM on Wednesday, March 1. **Posters must be removed by 12:30 PM on Thursday, March 2.**

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. The books booth will be staffed from 9:00 AM – 5:00 PM Monday through Thursday, and 9:00 AM - 11:30 AM on Friday. If a SIAM books representative is temporarily away from the booth, completed order forms and payment (credit cards are preferred) may be taken to the SIAM registration desk. The books table will close at 11:30 AM on Friday.

Table Top Displays

Association for Women in Mathematics
Cambridge University Press
Krell Institute
SIAM

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!

Conference Sponsors

Career Panel sponsored by:

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Comments?

Comments about SIAM meetings are encouraged! Please send to: Cynthia Phillips, SIAM Vice President for Programs (*vpp@siam.org*).

Get-togethers

Welcome Reception
Sunday, February 26
6:00 PM - 8:00 PM

Poster Sessions
Tuesday, February 28
4:30 PM - 6:30 PM

Wednesday, March 1
4:30 PM - 6:30 PM

Business Meeting
(open to SIAG/CSE members)
Thursday, March 2
6:20 PM – 7:20 PM
Complimentary beer and wine 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 personal electronic devices unattended. Please remember to turn off your cell phones and other devices 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 #SIAMCSE17.

SIAM's Twitter handle is @TheSIAMNews.

Prize Award Ceremony

On Thursday, March 2, 9:00-9:30 AM, the prize award ceremony will take place. The following prizes will be acknowledged and announced: SIAM/ACM Prize in Computational Science and Engineering, CSE17 Poster prizes and the Computational Engineering (BGCE) Student Paper Prizes.

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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:

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SIAM Activity Group on Computational Science and Engineering(SIAG/CSE)

www.siam.org/activity/cse

A GREAT WAY TO GET INVOLVED!

Collaborate and interact with mathematicians and applied scientists whose work involves computational science and engineering.

ACTIVITIES INCLUDE:

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

BENEFITS OF SIAG/CSE membership:

- Listing in the SIAG's online membership directory
- Additional $15 discount on registration at the SIAM Conference on Computational Science and Engineering (excludes student)
- Electronic communications about recent developments in your specialty
- Eligibility for candidacy for SIAG/CSE office
- Participation in the selection of SIAG/CSE officers

ELIGIBILITY:

- Be a current SIAM member.

COST:

- $15 per year
- Student members can join two activity groups for free!

SIAM Conference on
Computational Science and Engineering

February 27-March 3, 2017
Hilton Atlanta, Atlanta, Georgia, USA

2017-18 SIAG/CSE OFFICERS

Chair:	Hans De Sterck, Monash University
Vice-Chair:	Lorena Barba, George Washington University
Program Director:	Suzanne Shontz, University of Kansas
Secretary	Karen Devine, Sandia National Laboratories

TO JOIN:

SIAG/CSE: *my.siam.org/forms/join_siag.htm*

SIAM: *www.siam.org/joinsiam*

Invited Plenary Speakers

**** All Invited Plenary Presentations will take place in Grand Ballroom****

Monday, February 27

9:00 AM - 9:45 AM

IP1 Algorithmic Adaptations to Extreme Scale

David E. Keyes, *King Abdullah University of Science & Technology (KAUST), Saudi Arabia*

1:30 PM - 2:15 PM

IP2 Challenges for Climate and Weather Prediction in the Era of Exascale Computer Architectures: Oscillatory Stiffness, Time-Parallelism, and the Role of Long-Time Dynamics

Beth Wingate, *University of Exeter, United Kingdom*

Tuesday, February 28

8:15 AM - 9:00 AM

IP3 Ingredients for Computationally Efficient Solution of Large-Scale Image Reconstruction Problems

Misha E. Kilmer, *Tufts University, USA*

11:20 AM - 12:05 PM

IP4 Making Sense of our Universe with Supercomputers

Tom Abel, *Stanford University, USA*

Invited Plenary Speakers

**** All Invited Plenary Presentations will take place in Grand Ballroom****

Wednesday, March 1

8:15 AM - 9:00 AM

IP5 Multiscale modelling: Powerful Tool or Too Many Promises
Mikko Karttunen, *Eindhoven University of Technology, Netherlands*

11:20 AM - 12:05 PM

IP6 Title To Be Announced
Ann Almgren, *Lawrence Berkeley National Laboratory, USA*

Thursday, March 2

8:15 AM - 9:00 AM

IP7 Productive and Sustainable: More Effective Computational Science and Engineering
Michael Heroux, *Sandia National Laboratories, USA*

11:50 AM - 12:35 PM

IP8 Computational Science and Engineering Achievements in the Designing of Aircraft
Bruno Stoufflet, *Dassault Aviation, France*

Friday, March 3

8:15 AM - 9:00 AM

IP9 Stochastic Gradient Methods for Machine Learning
Jorge Nocedal, *Northwestern University, USA*

Minitutorials

***** All Minitutorials will take place in Ballroom C *****

Monday, February 27

10:15 AM - 11:55 AM

MT1 Version Control with Git- Part I

Organizer: **Randall LeVeque**, *University of Washington, USA*

2:25 PM - 4:05 PM

MT2 Version Control with Git- Part II

Organizer: **Randall LeVeque**, *University of Washington, USA*

Tuesday, February 28

9:10 AM - 10:50 AM

MT3 CSE Collaboration through Software: Improving Productivity and Sustainability- Part I

Organizer: **Lois Curfman McInnes,** *Argonne National Laboratory, USA*

1:30 PM - 3:10 PM

MT4 CSE Collaboration through Software: Improving Productivity and Sustainability- Part II

Organizer: **Lois Curfman McInnes,** *Argonne National Laboratory, USA*

Minitutorials

***** All Minitutorials will take place in Ballroom C *****

Wednesday, March 1

9:10 AM - 10:50 AM

MT5 Julia: Technical Computing made Fast, Flexible, and Easy
Organizer: **Alan Edelman,** *Massachusetts Institute of Technology and Julia Computing, USA*

1:30 PM - 3:10 PM

MT6 Exploring the Potential of the PRIMME Eigensolver
Organizer: **Andreas Stathopoulos,** *College of William & Mary, USA*

Thursday, March 2

10:00 AM - 11:40 AM

MT7 Interactive CSE with IPython and Jupyter- Part I
Organizer: **Min Ragan-Kelley**, *Simula Research Laboratory, Norway*

2:15 PM - 3:55 PM

MT8 Interactive CSE with IPython and Jupyter- Part II
Organizer: **Min Ragan-Kelley**, *Simula Research Laboratory, Norway*

Career Fair
Careers in Business, Industry, and Government

Monday, February 27

Part I: 10:15 AM - 11:55 AM
Part II: 2:25 PM - 4:05 PM
Part III: 4:35 PM - 6:15 PM
Room: Galleria

The career fair will feature representatives from nonacademic employers from industry and government. These representatives will be prepared to discuss with you the opportunities for internships, postdoctoral appointments and full-time jobs at their organizations.

The career fair will feature morning and afternoon sessions during which you will have the opportunity to speak with the representatives of the participating organizations. In addition to these sessions, there will be career panel over lunch and a professional development workshop and reception in the evening.

In order to maximize the value of your discussion, SIAM recommends that you take time beforehand to learn about the organizations that interest you.

SIAM is pleased to share the list of organizations that will participate in the 2017 Career Fair. This list is current at time of printing. The most up to date list of participants can be found at *http://www.siam.org/meetings/cse17/career.php*

Argonne National Laboratory
Department of Energy computational Science Graduate Fellowship (DOE CSGF)
IBM Research
Intelligent Light
KAUST
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
MathWorks
National Institute of Standards and Technology
NASA Langley Research Center
Naval Nuclear Laboratory
Oak Ridge National Laboratory
SigOpt
United Technologies Research Center

SIAM Presents is an audio-visual archive

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

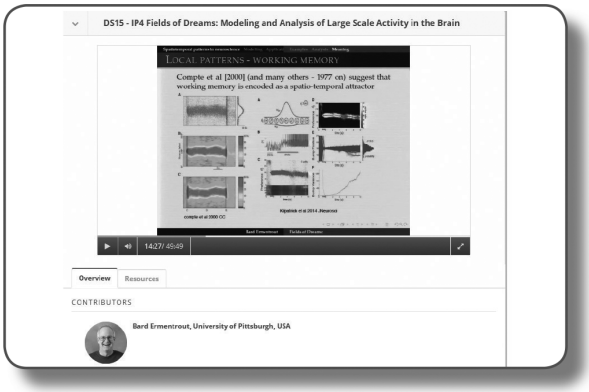
- **algebraic geometry**
- **atmospheric and oceanographic science**
- **computational science**
- **data mining**
- **geophysical science**
- **optimization**
- **uncertainty quantification and more…**

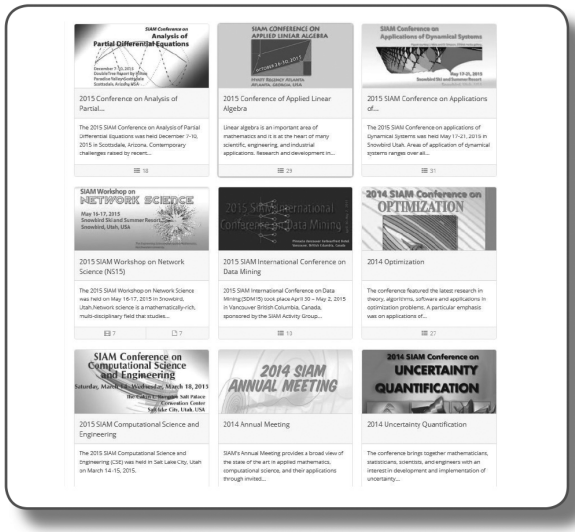
The collection, *Featured Lectures from our Archives*, includes audio and slides from more than 30 conferences since 2008, including talks by invited and prize speakers, select minisymposia, and minitutorials. Presentations from SIAM meetings are being added throughout the year.

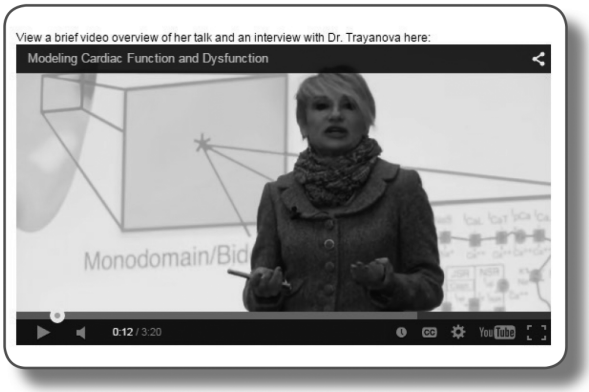
In addition you can view short video clips of speaker interviews from sessions at Annual Meetings starting in 2010.

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

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Program Schedule

SIAM Conference on Computational Science and Engineering

February 27-March 3, 2017
Hilton Atlanta, Atlanta, Georgia, USA

Sunday, February 26

Registration
1:00 PM-8:00 PM

Room:Foyer - 1st Fl

Welcome Reception
6:00 PM-8:00 PM

Room:Foyer - 2nd Fl

Monday, February 27

Registration
7:45 AM-5:00 PM

Room:Foyer - 1st Fl

Welcome Remarks
8:45 AM-9:00 AM

Room:Grand Ballroom - 2nd Fl

Monday, February 27

IP1

Algorithmic Adaptations to Extreme Scale
9:00 AM-9:45 AM

Room:Grand Ballroom - 2nd Fl

Chair: Omar Ghattas, University of Texas at Austin, USA

Algorithmic adaptations to use next-generation computers closer to their potential are underway. Instead of squeezing out flops – the traditional goal of algorithmic optimality, which once served as a reasonable proxy for all associated costs – algorithms must now squeeze synchronizations, memory, and data transfers, while extra flops on locally cached data represent only small costs in time and energy. After decades of programming model stability with bulk synchronous processing, new programming models and new algorithmic capabilities (to make forays into, e.g., data assimilation, inverse problems, and uncertainty quantification) must be co-designed with the hardware. We briefly recap the architectural constraints, then concentrate on two kernels that each occupy a large portion of all scientific computing cycles: large dense symmetric/Hermitian systems (covariances, Hamiltonians, Hessians, Schur complements) and large sparse Poisson/Helmholtz systems (solids, fluids, electromagnetism, radiation diffusion, gravitation). We examine progress in porting solvers for these kernels to the hybrid distributed-shared programming environment, including the GPU and the MIC architectures that make up the cores of the top scientific systems on the floor and on the books. How will the hierarchical solvers that lead in scalability (e.g., fast multipole, hierarchically low rank matrices, multigrid) map onto the more rigidly programmed and less reliably performant structures within a node?

David E. Keyes
King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Monday, February 27

Coffee Break

9:45 AM-10:15 AM

Room:Foyer - 2nd Fl

MT1

Version Control with Git-Part I

10:15 AM-11:55 AM

Room:Ballroom C - 2nd Fl

For Part 2 see MT2

Chair: Randall LeVeque, University of Washington, USA

The Git version control system is now widely used in the scientific computing community, not only for developing code (individually or collaboratively) but also for writing papers and grant proposals, sharing course materials with students and supporting group projects, and a host of other uses. The first part of this tutorial will introduce the basic concepts of Git and show how easy it is to get started using version control for your own work, on your own computer, as a good way to back up your work, keep track of changes you've made, revert to an earlier version if needed, and improve your ability to reproduce your own earlier work. The second part will cover more advanced concepts that are useful when using Git to collaborate with others, either privately or as part of an open source software community. We will cover branching, merging, forking, and the use of pull requests. We will also explore the tools available on GitHub, a popular collaboration site that hosts many open source projects. It is recommended that participants first install Git on their own laptops (see https://git-scm.com/book/en/v2/Getting-Started-Installing-Git) and create a free account on GitHub (see https://github.com/).

Randall LeVeque, University of Washington, USA; David I. Ketcheson, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Kyle T. Mandli, Columbia University, USA; Chris Vogl, University of Washington, USA

Monday, February 27

MS1

Career Fair: Careers in Business, Industry and Government - Part I of III

10:15 AM-11:55 AM

Room:Galleria

For Part 2 see MS30

The career fair will feature employers from business, industry and government. These representatives will be prepared to discuss with you the opportunities for internships, postdoctoral appointments and full-time jobs at their organizations.

Organizer: William G. Kolata
SIAM, USA

Organizer: Kristin O'Neill
SIAM, USA

The Most Current List of Participating Companies Is Available at *http://www.siam.org/meetings/cse17/career.php*

Monday, February 27

MS2

Inverse Problems Meet Big Data - Part I of III

10:15 AM-11:55 AM

Room:Grand Ballroom - 2nd Fl

For Part 2 see MS31

Inverse and big-data problems are pervasive in engineering and science. Though in past decades tremendous advances in both theories and computational algorithms for inverse problems have been made, addressing big-data issue is less common. Larger datasets implies more memory/time in processing/storing/loading. Since the amount of data we wish to process is only going to increase for the foreseeable future, there is a critical need for inverse algorithms, such as data fitting methods, that are computation- and data-scalable. This minisymposium aims to engage researchers from inverse problems and big data problems in discussions about central questions of big data inverse problems.

Organizer: Matthias Chung
Virginia Tech, USA

Organizer: Tan Bui
University of Texas at Austin, USA

Organizer: Farbod Roosta-Khorasani
University of California, Berkeley, USA

10:15-10:35 Title Not Available

George Biros, University of Texas at Austin, USA

10:40-11:00 Sketched Ridge Regression: Optimization and Statistical Perspectives

Shusen Wang, Alex Gittens, and Michael Mahoney, University of California, Berkeley, USA

11:05-11:25 Large Scale Fusion of Energy Resolved Compton Scatter and Attenuation-Based X-Ray Data for Materials Characterization

Eric L. Miller, Hamideh Rezaee, Brian Tracey, and Abdulla Desmal, Tufts University, USA

11:30-11:50 A Data Scalable Hessian/KKT Preconditioner for Large Scale Inverse Problems

Nick Alger, Umberto Villa, Tan Bui, and Omar Ghattas, University of Texas at Austin, USA

Monday, February 27

MS3

Recent Advances in Local, Adaptive, and Multilevel Uncertainty Quantification Methods for Large-Scale Scientific Computing - Part I of III

10:15 AM-11:55 AM

Room:Ballroom D - 2nd Fl

For Part 2 see MS32

Uncertainty quantification methods have seen tremendous use throughout the computational science community for enabling rigorous predictive simulation. In this minisymposium, recent advances in uncertainty quantification methods will be presented, focusing on local and adaptive methods applicable to problems involving localized behavior or discontinuities; multilevel methods exploiting hierarchies of fidelities for improved performance; and methods adapted for large-scale problems implemented on emerging extreme scale computer architectures.

Organizer: Eric Phipps
Sandia National Laboratories, USA

Organizer: Mohamed S. Ebeida
Sandia National Laboratories, USA

Organizer: Francesco Rizzi
Sandia National Laboratories, USA

10:15-10:35 A Novel Voronoi Piecewise Approach to Solve Stochastic PDEs

Mohamed S. Ebeida, Sandia National Laboratories, USA; Ahmad A. Rushdi, University of California, Davis, USA; Eric Phipps and Marta D'Elia, Sandia National Laboratories, USA

10:40-11:00 An Adaptive Method for Solving Stochastic Equations by Reduced Order Models Over Voronoi Cells

Wayne Isaac T. Uy, Haoran Zhao, and Mircea Grigoriu, Cornell University, USA

continued in next column

11:05-11:25 Practical Heteroskedastic Gaussian Process Modeling

Mickael Binois, Ecole des Mines de St Etienne, France; Robert Gramacy, Virginia Tech, USA; Mike Ludkovski, University of California, Santa Barbara, USA

11:30-11:50 Local Approximate Gaussian Processes for Large Computer Experiments

Robert Gramacy, Virginia Tech, USA

Monday, February 27

MS4

Eigenvectors and Decompositions of Structured Tensors

10:15 AM-11:55 AM

Room:202

Building a solid theoretical and computational foundation for hypermatrices and tensors is one of the current grand challenges in computational science and engineering and numerical multilinear algebra. Recently proposed generalizations of eigenvectors and low-rank decompositions have attractive uniqueness properties for specific tensor structures. Common structural assumptions are that the entries in the tensor are nonnegative or come from a higher-order Markov chain. These new methods have led to new computational algorithms and new applications in imaging and data science. The technologies and methods employed are quite diverse, drawing on stochastic processes, symbolic computation, and algebraic geometry. This minisymposium brings together diverse perspectives from numerical multilinear algebra and showcases a few ideas that demonstrate the richness of this research area. We will also have a focus on open problems, which are plentiful in this space.

Organizer: Austin Benson
Stanford University, USA

Organizer: David F. Gleich
Purdue University, USA

10:15-10:35 Spacey, Super Spacey, and Regenerative Spacey Random Walks

Austin Benson, Stanford University, USA

10:40-11:00 Transition Tensor of Spacey Random Walk for The Stationary Distribution of Polya Urn Process

Tao Wu, Purdue University, USA

continued on next page

11:05-11:25 On the Uniqueness of the Z_1-Eigenvector of Transition Probability Tensors
Kelly Pearson, Murray State University, USA

11:30-11:50 Symmetric Orthogonal Approximation to Symmetric Tensors and Its Applications to Image Reconstruction
Junjun Pan, Hong Kong Baptist University, Hong Kong

Monday, February 27

MS5

Extreme Scale Solvers - Part I of II

10:15 AM-11:55 AM

Room:203

For Part 2 see MS34

Exascale computers will exhibit billion-way parallelism. Computing on such extreme scale needs methods scaling perfectly with optimal complexity. This minisymposium combines talks on crucial aspects of extreme scale solving. The solver must be of optimal complexity, which is more an more severe with increasing problem size, and scale efficiently on extreme scales of parallelism. To that end, the minisymposium brings together talks on parallel adaptive multigrid methods in space and time, on nonlinear domain decomposition methods, as well as optimziation and uncertainty quantification techniques. Also, industrial applications and software aspects will be considered.

Organizer: Rolf Krause
Università della Svizzera italiana, Switzerland

Organizer: Gabriel Wittum
King Abdullah University of Science & Technology (KAUST), Saudi Arabia

10:15-10:35 ADVENTURE: Scalable Solvers for Industrial Applications
Hiroshi Kawai, Tokyo University of Science, Japan; Masao Ogino, Nagoya University, Japan; Ryuji Shioya, Toyo University, Japan; Tomonori Yamada and Shinobu Yoshimura, University of Tokyo, Japan

10:40-11:00 Identifying Structures in the Human Skin Using High Performance Shape Optimization Algorithms
Martin Siebenborn and Volker H. Schulz, University of Trier, Germany

11:05-11:25 Accelerating Groundwater Flow Simulation
Zeyao Mo, CAEP Software Center for High Performance Numerical Simulations, China

11:30-11:50 Parallel Tensor Arithmetic Applied to Multigrid Methods
Christian Loebbert, RWTH Aachen, Germany

Monday, February 27

MS6

Computational and Numerical Methods in Electronics - Part I if II

10:15 AM-11:55 AM

Room:204

For Part 2 see MS35

Research in electronics faces two challenges which are unfortunately often considered separate from each other: First, the rapid technological progress requires short simulation times for electronic devices with increasing geometric complexity. Such short simulation times can only be achieved through the development of new parallel algorithms since the serial performance of modern computing hardware stagnates. Second, sound numerical methods are required to accurately describe electronic transport at the discrete level. For example, important physical properties such as positivity and charge conservation need to be reflected in the numerics. This minisymposium aims at bridging the gap between both challenges by providing an interdisciplinary platform for physicists, numerical analysts and computational scientists.

Organizer: Karl Rupp
Freelance Computational Scientist, Austria

Organizer: Josef Weinbub
Christian Doppler Laboratory for High Performance TCAD, TU Wien, Austria

Organizer: Patricio Farrell
Weierstrass Institute, Germany

Organizer: Nella Rotundo
Weierstrass Institute, Germany

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Monday, February 27

MS6

Computational and Numerical Methods in Electronics - Part I if II

10:15 AM-11:55 AM

continued

10:15-10:35 Computational and Numerical Challenges in Semiconductor Process Simulation
Paul Manstetten, Vito Šimonka, Georgios Diamantopoulos, Lukas Gnam, and Alexander Makarov, Christian Doppler Laboratory for High Performance TCAD, TU Wien, Austria; Andreas Hössinger, Silvaco Europe Ltd., United Kingdom; *Josef Weinbub*, Christian Doppler Laboratory for High Performance TCAD, TU Wien, Austria

10:40-11:00 Electron Transport in Nanostructures: Physical Models and Numerical Methods
Massimo V. Fischetti and William Vandenberghe, University of Texas at Dallas, USA; Maarten Van de Put, University of Antwerp and IMEC, Belgium; Jingtian Fang, Vanderbilt University, USA; Shanmeng Chen, University of Texas at Dallas, USA

11:05-11:25 Modeling Spin-Dependent Phenomena for New Device Applications
Viktor Sverdlov, Josef Weinbub, and Siegfried Selberherr, TU Wien, Austria

11:30-11:50 Fast Reaction-Diffusion of Defects in Cadmium Telluride
Daniel Brinkman, San Jose State University, USA; Christian Ringhofer, Arizona State University, USA

Monday, February 27

MS7

Modeling and Computational Methods in Network Science and Applications - Part I of II

10:15 AM-11:55 AM

Room:205

For Part 2 see MS36

In recent years, there has been high demand for novel and accurate mathematical models, and fast, stable and scalable computational techniques to address problems emerging from applications on real-world networks, such as social media and power grids. In these applications, big data is often generated, collected, stored and/or processed in large-scale heterogeneous networks. New models and computational methods must tackle challenges of inhomogeneous structures of networks, randomness of dynamics, and noise in data. This minisymposium focuses on the recent advances of mathematical modeling and numerical methods as well as their applications in modern network science.

Organizer: Xiaojing Ye
Georgia State University, USA

Organizer: Honguyan Zha
Georgia Institute of Technology, USA

Organizer: Haomin Zhou
Georgia Institute of Technology, USA

10:15-10:35 Influence Prediction for Continuous-Time Information Propagation on Networks Using Graph-Based Fokker-Planck Equation
Xiaojing Ye, Georgia State University, USA

10:40-11:00 Walk-Based Centrality and Communicability Measures: Algorithms and Applications
Michele Benzi, Emory University, USA

11:05-11:25 Multilevel Model Reduction for Dynamic Power Grid Networks
Barry Lee, Southern Methodist University, USA

11:30-11:50 Dynamic Processes Over Information Networks: Representation, Modeling, Learning and Inference
Le Song, Georgia Institute of Technology, USA

Monday, February 27

MS8

Smooth, Reduced, Sparse -- Exploiting Structures for Surrogate Modeling in CSE - Part I of III

10:15 AM-11:55 AM

Room:206

For Part 2 see MS37

This minisymposium explores and highlights techniques that exploit structures in computationally expensive high-fidelity models to derive accurate low-cost surrogate models. A prominent example is projection-based model reduction, which exploits that states of the high-fidelity model can be approximated well in a reduced space of low dimension. Other methods exploit the smoothness of functions that are induced by the high-fidelity model (e.g., input-output and parameter-output maps), or sparsity of representations of the high-fidelity model outputs in well-chosen bases.

Organizer: Benjamin Peherstorfer
Massachusetts Institute of Technology, USA

Organizer: Gianluigi Rozza
SISSA-ISAS International School for Advanced Studies, Italy

10:15-10:35 Surrogate Modelling by Nonsymmetric Greedy Kernel Approximation
Bernard Haasdonk and Gabriele Santin, Universität Stuttgart, Germany

10:40-11:00 Structure-Preserving Nonlinear Model Reduction for Finite-Volume Models
Kevin T. Carlberg and Youngsoo Choi, Sandia National Laboratories, USA; Syuzanna Sargsyan, University of Washington, USA

continued on next page

11:05-11:25 Exploiting Low Tensor-Rank Structures in the Solutions to High-Dimensional Parametric PDE Problems

Peter Benner, Max Planck Institute for Dynamics of Complex Technical Systems, Germany; Sergey Dolgov, University of Bath, United Kingdom; Jan Heiland, Akwum Onwunta, and Martin Stoll, Max Planck Institute, Magdeburg, Germany

11:30-11:50 Optimal Model Reduction of Systems with Quadratic Nonlinearity

Peter Benner and Pawan Goyal, Max Planck Institute for Dynamics of Complex Technical Systems, Germany; *Serkan Gugercin*, Virginia Tech, USA

Monday, February 27

MS9

Hierarchically Rank-Structured Matrix Techniques - Part I of II

10:15 AM-11:55 AM

Room:209

For Part 2 see MS38

Rank-structured methods have demonstrated significant advantages in improving the efficiency and reliability of some large-scale computations and engineering simulations. These methods extend the fundamental ideas of multipole and panel-clustering methods to general non-local solution operators. While there exist various more or less closely related methods, the unifying aim of these methods is to explore efficient structured low-rank approximations, especially those exhibiting hierarchical or nested forms. In this minisymposium, we aim to present and exchange recent new developments such as efficient linear complexity algorithms, the construction of direct solvers for partial differential and integral equations, structured eigenvalue solutions, structured preconditioning, randomized algorithms, as well as implementation aspects.

Organizer: Sabine Le Borne

Hamburg University of Technology, Germany

Organizer: Jianlin Xia

Purdue University, USA

10:15-10:35 Hierarchical Matrices in Scattered Data Approximation

Sabine Le Borne, Hamburg University of Technology, Germany

10:40-11:00 $\mathcal{H}$-Matrix Accelerated Second Moment Analysis for Second Order {PDE}s

Juergen Doelz, Helmut Harbrecht, and Michael Peters, Universität Basel, Switzerland; Christoph Schwab, ETH Zürich, Switzerland

11:05-11:25 Stable Recurrences for Orthogonal Transformation of Givens-Weight and Block Givens-Weight Representations

Michael Stewart, Georgia State University, USA

11:30-11:50 Fast Bidirectional Solver for the High-Frequency Lippmann-Schwinger Equation

Leonardo Zepeda-Nunez and Hongkai Zhao, University of California, Irvine, USA

Monday, February 27

MS10

Monte Carlo and Ensemble Methods for Uncertainty Quantification

10:15 AM-11:55 AM

Room:210

For Part 2 see MS39

A common goal of uncertainty quantification is the calculation of probabilities, expected values, etc. of a random variable. Given a probability density function these quantities can be represented as integrals. Monte Carlo integration is frequently used to compute multidimensional integrals due to its dimensionally independent convergence. However, this convergence is often slow which is troublesome when the random variable involved is obtained from an expensive computational model or the event has complicated geometry. This minisymposium explores techniques for efficiently sampling stochastic space to compute multidimensional integrals with emphasis on ensemble model evaluations, efficient use of multifidelity models, and sample selection.

Organizer: Lindley C. Graham

Florida State University, USA

Organizer: Nan Jiang

Missouri University of Science and Technology, USA

10:15-10:35 A Fast Algorithm to Compute Flow Ensembles

Nan Jiang, Missouri University of Science and Technology, USA

10:40-11:00 Efficient Algorithms for MHD Simulation and Ensemble Calculations

Leo Rebholz and Muhammad Mohebujjaman, Clemson University, USA

11:05-11:25 From Inverses to Predictions: End-to-End UQ With MC Methods

Troy Butler, University of Colorado, Denver, USA

continued on next page

Monday, February 27

MS10

Monte Carlo and Ensemble Methods for Uncertainty Quantification

10:15 AM-11:55 AM

continued

11:30-11:50 Efficient Sampling Strategies for the Consistent Bayesian Approach for Solving Stochastic Inverse Problems

Tim Wildey, Sandia National Laboratories, USA; Troy Butler, University of Colorado, Denver, USA; John D. Jakeman, Sandia National Laboratories, USA

Monday, February 27

MS11

Integral Equation Methods for Particulate Flows - Part I of II

10:15 AM-11:55 AM

Room:211

For Part 2 see MS40

This minisymposium will focus on recent advances in the development and/or application of integral equation methods for low-Re viscous flow of drops, vesicles, rigid particles or other particulate suspensions.

Organizer: Shravan Veerapaneni

University of Michigan, USA

10:15-10:35 Contact-Aware Simulations of Particulate Stokesian Suspensions

Abtin Rahimian, Libin Lu, and Denis Zorin, Courant Institute of Mathematical Sciences, New York University, USA

10:40-11:00 A New Boundary Integral Equation Formulation for Vesicle Electrohydrodynamics

Bowei Wu and Shravan Veerapaneni, University of Michigan, USA

11:05-11:25 An Integral Equation Method for 3D Surfactant-Covered Drops

Chiara Sorgentone, KTH Royal Institute of Technology, Sweden

11:30-11:50 A Unified Approach to Periodization of Fast Algorithms for Laplace and Stokes Problems

Alex H. Barnett, Dartmouth College and Simons Foundation, USA; Gary Marple and Shravan Veerapaneni, University of Michigan, USA; Lin Zhao, INTECH, USA

Monday, February 27

MS12

Advances in Cut Cell Discretizations: Accuracy, Stability, and Applications

10:15 AM-11:55 AM

Room:212

Ongoing research into cut cell methods have improved their applicability for solving PDEs in complex geometries. Starting with a regular grid, these methods treat cells near the boundary with modified finite difference, finite volume and other discretizations. Thus they can more easily represent complex and moving geometries, without requiring changes to a global mesh, across a wide range of applications. Challenges include gaps in theoretical underpinnings for higher-order methods, issues due to arbitrarily small cells, and the programming complexity that arises with cell merging and other stabilization techniques. This minisymposium will highlight recent algorithmic advances and a variety of science domain applications.

Organizer: Hans Johansen

Lawrence Berkeley National Laboratory, USA

10:15-10:35 Higher-Order Cut Cell Finite Volume Discretizations: Theory and Applications

Hans Johansen, Lawrence Berkeley National Laboratory, USA

10:40-11:00 Inverse Lax–Wendroff Procedure for Numerical Boundary Conditions of Convection–Diffusion Equations

Jianfang Lu, Beijing Computational Science Research Center, China; Jinwei Fang, Harbin Institute of Technology, China; Sirui Tan and Chi-Wang Shu, Brown University, USA; Mengping Zhang, University of Science and Technology of China, China

continued on next page

11:05-11:25 Application of a High-Order Adaptive Cut-Cell Method to Complex Moving Deformable Boundary Problems

Balaji Muralidharan and Suresh Menon, Georgia Institute of Technology, USA

11:30-11:50 A Moving Boundary Cut Cell Approach for Incompressible Euler with a Free Surface

Curtis Lee, Duke University, USA; Dan Graves, Hans Johansen, and Amneet Pal S. Bhalla, Lawrence Berkeley National Laboratory, USA; John Dalbow, Duke University, USA

Monday, February 27

MS13

Recent Advance on Numerical Methods for Quantum Problems - Part I of III

10:15 AM-11:55 AM

Room:213

For Part 2 see MS42

Quantum problems have numerous applications in quantum physics and chemistry, plasma and particle physics, material sciences, semiconductor theory, rarefied gas theory, Bose-Einstein condensation, nonlinear optics, erc. The typical models include nonlinear Schroedinger equation (NLS), Dirac equation, Klein-Gordon equation, density fucntional theory, quantum Boltzmann equation, etc. The purpose of this minisymposium is to provide a platform for the researchers in the field to present recent work on the numerical analysis, numerical methods and simulation for these quantum problems, to exchange idea and to discuss future directions in the field.

Organizer: Yongyong Cai

Beijing Computational Science Research Center, China

10:15-10:35 Numerical Method for the Dirac Equation in the Nonrelativistic Limit Regime

Yongyong Cai, Beijing Computational Science Research Center, China

10:40-11:00 Numerical Analysis of Finite Temperature DFT

Huajie Chen, Beijing Normal University, China

11:05-11:25 A Fast Deterministic Solver for the Schrodinger-Quantum Boltzmann System

Jingwei Hu, Purdue University, USA

11:30-11:50 Towards a Mathematical Understanding of Surface Hopping Algorithms

Zhennan Zhou and Jianfeng Lu, Duke University, USA

Monday, February 27

MS14

Neutrino Transport Methods in Astrophysics

10:15 AM-11:55 AM

Room:214

For Part 2 see MS43

Core-collapse supernovae (CCSNe) and neutron star mergers are cataclysmic astrophysical events responsible for heavy element synthesis and the emission of photon, neutrino, and gravitational wave signals. They have long been targets of instruments covering most of the electromagnetic spectrum, and more recently of neutrino and gravitational wave detectors (e.g. IceCube and LIGO). Harvesting insights into the physical processes driving these events from this wealth of data relies heavily on sophisticated models requiring extreme-scale, high-fidelity computing. These models solve a coupled system of equations for self-gravity, magneto-hydrodynamics, and neutrino transport. For example, about 99% of the gravitational energy released during a CCSN is radiated away in the form of neutrinos, which are likely a major driver of the supernova explosion. However, neutrino-matter interactions occur under non-equilibrium conditions (neutrinos are semi-transparent to the stellar fluid) and a description based on the Boltzmann transport equation is warranted. As a six-dimensional phase-space problem, our ability to model these astrophysical events with satisfactory realism relies on advances in multi-physics and multi-scale algorithms, novel discretization techniques, fast solvers, and sustainable scientific software. The goal of this minisymposium is to bring together researchers working on topics of relevance to neutrino transport modeling to discuss recent work and exchange ideas.

Organizer: Eirik Endeve

Oak Ridge National Laboratory, USA

continued on next page

Monday, February 27

MS14

Neutrino Transport Methods in Astrophysics

10:15 AM-11:55 AM

continued

Organizer: Christian Cardall
Oak Ridge National Laboratory, USA

10:15-10:35 Radiation Hydrodynamics in GenASiS
Christian Cardall, Oak Ridge National Laboratory, USA

10:40-11:00 Two-Moment Neutrino Transport Coupled to Relativistic MHD for Stellar Core Collapse
Martin Obergaulinger and Miguel Angel Aloy, University of Valencia, Spain

11:05-11:25 Multi-Dimensional Boltzmann-Neutrino-Radiation-Hydrodynamic Simulations in Core Collapse Supernovae
Hiroki Nagakura, California Institute of Technology, USA; Wakana Iwakami, Yukawa Institute for Theoretical Physics, Kyoto, Japan; Shun Furusawa, J.W. Goethe-Universität, Germany; Kohsuke Sumiyoshi, Numazu National College of Technology, Japan; Shoichi Yamada, Waseda University, Japan; Hideo Matsufuru, High Energy Accelerator Research Organization, Japan; Akira Imakura, University of Tsukuba, Japan; Sherwood Richers and Christian Ott, California Institute of Technology, USA

11:30-11:50 Positivity Limiters on the Filtered P_N Method for Linear Transport Equations
Ming Tse P. Laiu and Cory Hauck, Oak Ridge National Laboratory, USA

Monday, February 27

MS15

Efficiency of High-Order Methods on the 2nd Generation Intel Xeon Phi Processor - Part I of II

10:15 AM-11:55 AM

Room:215

For Part 2 see MS44

In Summer 2016 the 2nd generation Intel Xeon Phi Processor (Knights Landing) was released. It will be the computational heart of many future supercomputing installations. Examples are the DoE-machines "Trinity-II", "Cori-II" and "Theta", "Stampede-2" of NSF, or the future 25 PFLOPS machine "Oakforest-PACS" in Japan. The 2nd generation of the Xeon Phi processor combines the computational power of accelerator-based machines with the traditional approach of homogeneous high performance computing. From an application viewpoint, many research articles in the last years have proven that high-order methods require the computational power of modern supercomputers. However, it is a challenging engineering problem to enable complex software packages on manycore architectures. This minisymposia brings together researchers working on efficient implementations of scalable higher-order solvers. Of particular interest are applications which are known to require exascale computing resources in future, such as computational fluid dynamics, electro-magnetics and seismic simulations, as well as weather forecasting. Due to the broad spectrum of applications, this MS aims at identifying common algorithmic patterns of efficient high-order methods. Additionally, the comparison of different numerical approaches (e.g. CG vs. DG) will allow to identify best practices and an early performance/ease-of-use estimator when leveraging Intel Xeon Phi systems at scale.

continued in next column

Organizer: Alexander Heinecke
Intel Corporation, USA

Organizer: Alexander Breuer
University of California, San Diego, USA

10:15-10:35 PyFR and GiMMiK on Intel KNL: Performance, Scalability, and Applications
Freddie D. Witherden, Stanford University, USA; Jin Seok Park, Imperial College London, United Kingdom; Alexander Heinecke, Intel Corporation, USA; Paul Kelly and Peter E. Vincent, Imperial College London, United Kingdom; Antony Jameson, Stanford University, USA

10:40-11:00 H-to-P Efficiently: The Use of Collections with Accelerators Within Nektar++
David Moxey and Chris Cantwell, Imperial College, United Kingdom; Mike Kirby, University of Utah, USA; Spencer Sherwin, Imperial College, United Kingdom

11:05-11:25 Spectral Element Simulations of Turbulence on ALCF Theta
Paul Fischer, University of Illinois at Urbana-Champaign, USA

11:30-11:50 Performance Evaluation of a Very Efficient High-Order Accurate Imex Solver for Incompressible Fluid Dynamics on Intel Xeon Phi
Matteo Parsani, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Monday, February 27

MS16

Automatic Code Generation for Simulation and Optimization - Part I of II

10:15 AM-11:55 AM

Room:216

For Part 2 see MS45

Scientific computing plays an ever increasing role in understanding complex physical processes and computer simulations are nowadays an indispensable tool in many fields and applications. Recent trends with respect to creating and maintaining high fidelity simulation codes for partial differential equations governing such problems are high level languages and automatic code generation. Being able to postulate a problem in a programming paradigm, which is both close to the mathematical problem description and can be processed by a computer, naturally makes understanding, developing and maintaining complex codes much easier. Transitioning to solving optimization problems is the next natural step. With the advent of high level domain specific programming languages such as UFL, it only nowadays becomes feasible to create unified code generation approaches for the primal and adjoint problem, where the differentiation tool has information available about the nature of the primal problem and the meaning of the instructions and variables it is currently processing, thereby creating a hybridized optimization framework between the continuous and discrete approach automatically. With these developments in mind, the aim of this minisymposium is to bring together the various recent trends in code generation for simulation and optimization with the intention to foster new structure exploiting hybridization strategies.

continued in next column

Organizer: Stephan Schmidt
Universität Würzburg, Germany

Organizer: Nicolas R. Gauger
Technische Universität Kaiserslautern, Germany

10:15-10:35 Automatic Generation of Shape Derivatives and Hessians

Stephan Schmidt, Universität Würzburg, Germany

10:40-11:00 Procedurally Generated Shape Hessians and Their Computation Using Fenics

Edwin Mai, Universität der Bundeswehr München, Germany; Stephan Schmidt, Universität Würzburg, Germany

11:05-11:25 Hessian Approximation Using Operator Symbols

Jonas Kusch, RWTH Aachen University, Germany; Nicolas R. Gauger, Technische Universität Kaiserslautern, Germany; Stephan Schmidt, Universität Würzburg, Germany

11:30-11:50 Different Taping Strategies for AD-based Adjoints Analyzed for SU2

Max Sagebaum, Nicolas R. Gauger, and Tim Albring, Technische Universität Kaiserslautern, Germany

Monday, February 27

MS17

Advances in MCMC and Related Sampling Methods for Large-Scale Inverse Problems - Part I of II

10:15 AM-11:55 AM

Room:217

For Part 2 see MS46

Inverse problems convert indirect measurements into useful characterizations of the parameters of a physical system. Parameters are typically related to indirect measurements by a system of partial differential equations (PDEs), which are complicated and expensive to evaluate. Available indirect data are often limited, noisy, and subject to natural variation, while the unknown parameters of interest are often high dimensional, or infinite dimensional in principle. Solution of the inverse problem, along with prediction and uncertainty assessment, can be cast in a Bayesian setting and thus naturally tackled with Markov chain Monte Carlo (MCMC) and other posterior sampling methods. However, designing scalable and efficient sampling methods for high dimensional inverse problems that involve expensive PDE evaluations poses a significant challenge. This minisymposium presents recent advances in sampling approaches for large scale inverse problems.

Organizer: Tiangang Cui
Monash University, Australia

Organizer: Youssef M. Marzouk
Massachusetts Institute of Technology, USA

Organizer: Tan Bui-Thanh
University of Texas at Austin, USA

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Monday, February 27

MS17

Advances in MCMC and Related Sampling Methods for Large-Scale Inverse Problems - Part I of II

10:15 AM-11:55 AM

continued

10:15-10:35 Estimating Large-Scale Chaotic Dynamics

Heikki Haario, Lappeenranta University of Technology, Finland

10:40-11:00 Triple Model Reduction for Efficient Bayesian Inversion

Vishwas Rao and Tan Bui-Thanh, University of Texas at Austin, USA

11:05-11:25 Advances in Generalised Metropolis-Hastings Algorithms

Ben Calderhead, Imperial College London, United Kingdom

11:30-11:50 Bayesian Inverse Problems with Infinitely-Divisible Priors

Bamdad Hosseini, Simon Fraser University, Canada

Monday, February 27

MS18

Algorithms and Libraries for Tensor Contractions - Part I of II

10:15 AM-11:55 AM

Room:218

For Part 2 see MS47

Tensors and tensor contractions are the multi-dimensional generalization of matrices and matrix products, respectively. They arise in a multitude of disciplines and applications, ranging from theoretical physics to quantum chemistry and machine learning. Interestingly, while the performance of the kernels for matrix-products (GEMM) is typically excellent, that of tensor contractions is often far from optimal. The difference is due to a number of factors, including the sheer size of the tensors, the suboptimal memory access patterns, the increased complexity to achieve locality, and possibly a low arithmetic intensity. This minisymposium is devoted to algorithms and libraries for the efficient calculation of tensor contractions. The existing approaches can be loosely classified in three categories: nested-loops, transpose-transpose-GEMM-transpose, and loops-over-GEMMs. With these eight talks, we bring together experts from all three categories, presenting a thorough overview of the state of the art in the field of high-performance tensor contractions.

Organizer: Paolo Bientinesi

RWTH Aachen University, Germany

10:15-10:35 TCCG: Tensor Contraction Code Generator

Paul Springer and Paolo Bientinesi, RWTH Aachen University, Germany

10:40-11:00 Practical Algorithms for Large Tensor Computations

Evgeny Epifanovsky, Q-Chem, Inc., USA

11:05-11:25 Loop Fusion to Optimize Sequences of Tensor Contractions

P. (Saday) Sadayappan and Samyam Rajbhandari, Ohio State University, USA; Karol Kowalski and Sriram Krishnamoorthy, Pacific Northwest National Laboratory, USA; Fabrice Rastello, Inria, France

11:30-11:50 Tensors and the Power of Imagination

Devin Matthews, University of Texas at Austin, USA

continued in next column

Monday, February 27

MS19

Applications and Computational Strategies for Finite Element Computations using LibMesh - Part I of II

10:15 AM-11:55 AM

Room:219

For Part 2 see MS48

The development of the libMesh finite element library began over a decade ago in order to support adaptive mesh refinement on unstructured grids for finite element simulations of complex applications. It has grown to support hundreds of users across the world, has been used and scaled on large parallel supercomputers, and enabled the study of a wide variety of finite element computations. This minisymposium aims to bring together users and developers of the libMesh finite element library to discuss the latest developments in the library, frameworks supported by the libMesh, and applications enabled by the libMesh infrastructure.

Organizer: Paul Bauman
State University of New York at Buffalo, USA

Organizer: Alvaro Coutinho
Federal University of Rio de Janerio, Brazil

Organizer: John W. Peterson
Idaho National Laboratory, USA

Organizer: Roy Stogner
University of Texas at Austin, USA

10:15-10:35 LibMesh: Past, Present, and Future

Roy Stogner, University of Texas at Austin, USA

10:40-11:00 Scalable Parallel Implementation of a Coupling Scheme Using LibMesh

Regis Cottereau, CNRS, CentraleSupelec, Université Paris-Saclay, France; Thiago Milanetto Schlittler, CentraleSupélec, France

continued in next column

11:05-11:25 Sedimentation and Deposition Simulation with LibMesh

Jose J. Camata and Andre Rossa, Federal University of Rio de Janerio, Brazil; Adriano Cortes, UNRIO, Brazil; Alvaro Coutinho, COPPE/Universidade Federal do Rio e Janeiro, Brazil

11:30-11:50 A Monolithic Approach to Numerical Simulation of Airflow in the Lungs

James P. Mbewu, University of Oxford, United Kingdom

Monday, February 27

MS20

Toward Resiliency via Numerical Remedies - Part I of II

10:15 AM-11:55 AM

Room:220

For Part 2 see MS49

Future extreme scale systems are expected to suffer more frequent hard faults and soft error resulting from the unprecedented scale of parallelism. Combined with the technology trend such as the imbalance between computing and I/O throughput and a tight power budget in the system operations, the traditional hardware-level redundancy and checkpoint restart may not be a feasible solution. Although, every layer of the systems should address these faults to mitigate their impact in holistic manners, we will focus in this minisymposium the deficiencies from a algorithm and applications viewpoint.

Organizer: Keita Teranishi
Sandia National Laboratories, USA

Organizer: Luc Giraud
Inria, France

Organizer: Emmanuel Agullo
Inria, France

Organizer: Michael Heroux
Sandia National Laboratories, USA

10:15-10:35 Using Error Estimates In Resiliency

Pierre-Louis Guhur, Ecole Normale Superieur de Cachan, France; Franck Cappello and Emil M. Constantinescu, Argonne National Laboratory, USA

10:40-11:00 Soft Error Resilience in Big Data Kernels: An Algorithmic Approach

Lu Peng, Sui Chen, Travis LeCompte, and Walker Legrand, Louisiana State University, USA

11:05-11:25 A Self-Correcting Connected Components Algorithm

Piyush Sao and Richard Vuduc, Georgia Institute of Technology, USA

11:30-11:50 Data Compression for Checkpoint Optimization

Jon Calhoun, University of Illinois at Urbana-Champaign, USA; Franck Cappello, Argonne National Laboratory, USA; Luke Olson and Marc Snir, University of Illinois at Urbana-Champaign, USA

Monday, February 27

MS21

Scientific Workflow Environment toward Extreme-Scale Computing - Part I of II

10:15 AM-11:55 AM

Room:Crystal AF - 1st Fl

For Part 2 see MS50

The continuous progress in high performance and cloud computing technology has enabled scientists and engineers to understand multi-scale and multi-physics phenomena at unprecedented complexity and scale. Today, many science and engineering computations are comprised with multiple application programs including compute-intensive simulations, data analytics and visualization. For such application couplings, scientific workflow software is essential to express the interactions among these programs transparently and seamlessly connect them in platform independent manner. In addition to such couplings, the workflow provides a steerings to use to dynamically control program executions and input parameter settings to permit the users to investigate the point of their interest with a better focus. In this minisymposium, we discuss the techniques and challenges of scientific-workflow for future extreme scale computing environment, including performance, scalability, resilience, and usability issues.

Organizer: Keita Teranishi

Sandia National Laboratories, USA

Organizer: Martin Schulz

Lawrence Livermore National Laboratory, USA

10:15-10:35 Challenges in Managing Scientific Workflows in Heterogeneous Environments

Ewa Deelman, University of Southern California, USA

continued in next column

10:40-11:00 Towards Executing Dynamic and Adaptive Application Workflows on Heterogeneous Infrastructure Using Pilot-Abstractions

Mark Santcroos and *Shantenu Jha*, Rutgers University, USA

11:05-11:25 Implementing Multi-Scale Simulation Workflows with COMPS

Raül Sirvent and Rosa M. Badia, Barcelona Supercomputing Center, Spain

11:30-11:50 The Uintah - VisIt Coupled Workflow

Allen Sanderson, Alan Humphrey, John A. Schmidt, and Martin Berzins, University of Utah, USA

Monday, February 27

MS22

Model Discrepancy and Model Form Error: Bayesian Approaches

10:15 AM-11:55 AM

Room:Crystal CD - 1st Fl

For Part 2 see MS51

Model discrepancy is defined as the difference between model predictions and experimental data, sometimes called "model form error" or "structural model error". There are a variety of approaches being developed, including formulations that represent discrepancy explicitly using, for example, Gaussian processes or polynomial chaos expansions, as well as implicit formulations in which "model correction" terms are determined concurrently with the solution of a set of partial differential equations. Approaches that are Bayesian or non-Bayesian in nature, along with those supported by machine learning principles, may be used to estimate model discrepancy. This minisymposium encompasses the Bayesian approaches and is meant to foster discussion of the various methods.

Organizer: Laura Swiler

Sandia National Laboratories, USA

Organizer: Kathryn Maupin

Sandia National Laboratories, USA

10:15-10:35 Model Discrepancy and Influenza Forecasting: A Bayesian Hierarchical Modeling Approach

David Osthus and James Gattiker, Los Alamos National Laboratory, USA

10:40-11:00 Model Error and Statistical Calibration of Physical Models

Habib N. Najm, Khachik Sargsyan, and Xun Huan, Sandia National Laboratories, USA

11:05-11:25 Bayesian Calibration of Simulators with Structured Discretization Uncertainty

Matthew T. Pratola and *Oksana A. Chkrebtii*, Ohio State University, USA

11:30-11:50 Model Error in CO2 Retrieval from Satellite Measurements

Jenny Brynjarsdottir, Case Western Reserve University, USA; Jonathan Hobbs and Amy Braverman, California Institute of Technology, USA

Monday, February 27

MS23

Stochastic PDE-Constrained Optimization and Applications - Part I of II

10:15 AM-11:55 AM

Room:301

For Part 2 see MS52

Engineering decisions are often formulated as optimization problems constrained by partial differential equations (PDEs). Unfortunately, these governing PDEs are typically fraught with uncertainties including input parameters estimated from noisy and incomplete data, unknown initial and boundary conditions, and unverifiable modeling assumptions. Thus, the need to make robust or risk-averse decisions pervades nearly all engineering applications including, e.g., optimal control and design, and inverse problems. Due to the array of computational and theoretical difficulties associated with these problems, it is critical to develop new techniques in stochastic programming, PDE-constrained optimization and tensor methods. The goal of this multi-part minisymposium is to showcase new research in these areas with application to PDE-constrained optimization under uncertainty.

Organizer: Drew P. Kouri

Sandia National Laboratories, USA

Organizer: Thomas M. Surowiec

Philipps-Universität Marburg, Germany

10:15-10:35 Time Consistency of Multistage Stochastic Programs

Alexander Shapiro, Georgia Institute of Technology, USA

10:40-11:00 Measures of Residual Risk with Connections to Regression, Risk Tracking, Surrogate Models, and Ambiguity

Johannes O. Royset, Naval Postgraduate School, USA

11:05-11:25 Surrogate Models For Characterizing Tail Statistics Of Systems Governed By PDEs

Stan Uryasev and Giorgi Pertaia, University of Florida, USA

11:30-11:50 Risk-Averse PDE-Constrained Optimization

Thomas M. Surowiec, Philipps-Universität Marburg, Germany; Drew P. Kouri, Sandia National Laboratories, USA

Monday, February 27

MS24

Advances in Enabling Quantification of Uncertainty in Physical Systems (EQUiPS)– Part I of II

10:15 AM-11:55 AM

Room:302

For Part 2 see MS53

Uncertainty quantification (UQ) is key for achieving validated predictive computations in a wide range of complex scientific and engineering applications. However, many fundamental challenges still remain in trying to build effective predictive models in engineering design of large, multi-physics and multi-scale physical systems. Existing computational and theoretical approaches and methodologies cannot adequately handle uncertainty emerging from high dimensional input parameter spaces, model form discrepancies, and random conditions in the operating environment of these systems. This minisymposium intends to explore and present advances at the forefront of research in these topics, ranging from highly efficient for both "forward" and "inverse" UQ algorithms to novel physics-based methodologies to capture model form uncertainty, leading to robust and dynamic decision-making frameworks for design under uncertainty. Topics include: Entropy metrics to measure model errors, multi-fidelity information fusion algorithms to quantify failure and rare events, new methods for likelihood estimation in Bayesian inference for inverse problems, and optimal control and design of turbulent flow systems under uncertainty.

Organizer: Habib N. Najm

Sandia National Laboratories, USA

Organizer: Fariba Fahroo

Air Force Office of Scientific Research, USA

continued in next column

10:15-10:35 From Data to Optimization Under Uncertainty: A Scalable Framework for Bayesian Inversion and Optimal Control of Random PDEs with Application to Turbulent Flows

Peng Chen, *Omar Ghattas*, Robert D. Moser, Todd A. Oliver, and Umberto Villa, University of Texas at Austin, USA

10:40-11:00 Model Error Quantification in Turbulent Combustion Computations

Khachik Sargsyan, Xun Huan, Zachary Vane, Guilhem Lacaze, Joseph C. Oefelein, and Habib N. Najm, Sandia National Laboratories, USA

11:05-11:25 Derivative-Free Constrained Stochastic Optimization of a Scramjet, Using SNOWPAC

Friedrich Menhorn, Technische Universität München, Germany; *Florian Augustin* and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

11:30-11:50 Numerical Simulation of Stochastic Navier-Stokes Equations Under High-Dimensional Random Forcing

Hessam Babaee, Massachusetts Institute of Technology, USA; George E. Karniadakis, Brown University, USA

Monday, February 27

MS25

Direct and Inverse Problems in Numerical Modeling of Cardiac Electrophysiology

10:15 AM-11:55 AM

Room:303

For Part 2 see MS54

Numerical cardiac electrophysiology has been developed for quantitatively understanding the dynamics of potential propagation in the heart. Notwithstanding the progressive refinement of models and methods, several challenges are still on. (1) The description of specific features (e.g. cardiac fibers) still requires modeling developments; (2) the patient specific perspective demands the efficient solution of inverse parameter estimation problems. This Minisymposium gathers mathematicians, physicists and engineers working on different sides of the problem for reliably solving both direct and inverse problems in electrophysiology. Modeling/ computational aspects, uncertainty quantification, validation and the point of view of clinicians will be represented. Supported by NSF.

Organizer: Alessandro Veneziani

Emory University, USA

Organizer: Flavio H. Fenton

Georgia Institute of Technology, USA

10:15-10:35 GPU Simulations of Heart Dynamics Close to Real Time and Over the Internet

Flavio H. Fenton and Abouzar Kaboudian, Georgia Institute of Technology, USA

10:40-11:00 Using Data Assimilation to Reconstruct Cardiac Electrical Dynamics

Elizabeth M. Cherry and Matthew J. Hoffman, Rochester Institute of Technology, USA; Nicholas LaVigne, Cornell University, USA; Nathan Holt and Darby Cairns, Rochester Institute of Technology, USA

11:05-11:25 An Approach to Estimating the Probability of Calcium-Induced Arrhythmias in Cardiac Cells and Tissues and Their Dependence on System Parameters

Raimond Winslow, Johns Hopkins University, USA

11:30-11:50 Cardiac Electrophysiology: The Clinical Perspective (The Greatest Gaps in Heart Rhythm Analysis: A Clinical Cardiac Electrophysiologist's Perspective on Atrial Fibrillation

Michael Lloyd, Iravanian Shahriar, and Jonathan Langberg, Emory University, USA

continued in next column

Monday, February 27

MS26

Advances in Computational Methods for Multiphysics Problems - Part I of II

10:15 AM-11:55 AM

Room:304

For Part 2 see MS55

There are many applications of multiphysics problems in material science, physics and mathematical biology. Modeling and simulating those problems, such as fluid structure interaction and conjugate heat transfer, have attracted considerable attentions from many researchers in recent years. This minisymposium aims to bring researchers together to discuss the state of the art methods and algorithms, and to share the numerical challenges in the various areas.

Organizer: Longfei Li

Rensselaer Polytechnic Institute, USA

Organizer: Qi Tang

Rensselaer Polytechnic Institute, USA

10:15-10:35 Added-Mass Partitioned (AMP) Algorithm for the Deforming Beam and Fluid Interaction

Longfei Li, Rensselaer Polytechnic Institute, USA

10:40-11:00 A High-Resolution Method for a Multi-Scale Model of Heterogeneous Explosives

Donald W. Schwendeman and Ashwani K. Kapila, Rensselaer Polytechnic Institute, USA

11:05-11:25 Fast and Adaptive Partitioned Methods for Unsteady Thermal Fluid Structure Interaction

Philipp Birken and Azahar Monge Sanchez, Lund University, Sweden

11:30-11:50 Coupling Requirements for Multi-Physics Problems

Fatemeh Ghasemi and Jan Nordström, Linköping University, Sweden

Monday, February 27

MS27

Recent Advances of Modeling and Computational Techniques in Biological Engineering - Part I of II

10:15 AM-11:55 AM

Room:305

For Part 2 see MS56

Mathematical modeling and computations are powerful tools for understanding the complex biological systems in bioengineering. Development of novel mathematical representations and robust computational techniques are critical for analyzing these systems. Recently, several successful attempts have been made for simulating complex biological processes like metabolic pathways, gene regulatory networks, cell signaling pathways, ion channels, cell dynamics, tumor growth, tissue engineering and biofabrication, etc. These computational-extensive models have not only reproduced experimentally verifiable phenomena, but also provided valuable insights for discovering mechanisms of the complex biological systems. This minisymposium will showcase recent progresses in developing efficient modeling and computational approaches for understanding various biological systems and their potential applications in bioengineering.

Organizer: Yi Sun

University of South Carolina, USA

Organizer: Shixin Xu

University of California, Riverside, USA

Organizer: Jia Zhao

University of North Carolina at Chapel Hill, USA

10:15-10:35 Modeling Leader and Follower in Cancer Invasion

Yi Jiang and Sean Keeler, Georgia State University, USA; Jessica Konen and Adam Marcus, Emory University, USA

10:40-11:00 Crawling and Turning of Cells in a Minimal Reaction-Diffusion Model

Yanxiang Zhao, George Washington University, USA; Brian Camley and Bo Li, University of California, San Diego, USA; Herbert Levine, Rice University, USA; Wouter-Jan Rappel, University of California, San Diego, USA

11:05-11:25 Stochastic Dynamics of 3D Vesicles in Viscous Flows

Kai Liu, University of California, Irvine, USA; Shuwang Li, Illinois Institute of Technology, USA; John Lowengrub, University of California, Irvine, USA

11:30-11:50 Multi-Scale Modeling and Simulation of the Growth of Bacterial Colony with Cell-Cell Mechanical Interactions

Hui Sun, University of California, San Diego, USA

continued in next column

Monday, February 27

MS28

Parallel Frameworks and Libraries for Tree-Structured Grids - Part I of II

10:15 AM-11:55 AM

Room:221

For Part 2 see MS57

Tree-structured computational grids have become more and more popular for various types of scientific simulations due to their advantages both in terms of fully-flexible local adaptivity and their tree-structure. The big challenges in using such grids in existing applications are 1) the effort to integrate the new grid type in a minimally-invasive while ensuring that the application inherits the advantages of the grid type in terms of memory requirements and 2) the realization of complex (and moving) geometries in the inherently Cartesian grid structure. The minisymposium presents and discusses solutions provided in frameworks and libraries addressing these two challenges.

Organizer: Miriam Mehl

Universität Stuttgart, Germany

Organizer: Carsten Burstedde

Universität Bonn, Germany

10:15-10:35 Tree-Structured Grids – Approaches for Storage, Data Access, and Discretization

Carsten Burstedde, Universität Bonn, Germany; Miriam Mehl, Universität Stuttgart, Germany

10:40-11:00 Using Voxel Meshes on Octrees for High-Fidelity Simulations with Complex Geometries

Sabine P. Roller and Harald Klimach, Universität Siegen, Germany

11:05-11:25 Parallel Forest-of-Trees Algorithms for Tetrahedral and Hexahedral AMR

Johannes Holke and Carsten Burstedde, Universität Bonn, Germany

11:30-11:50 Fast Integral Equation Solver for Elliptic PDEs in Complex Geometries

Dhairya Malhotra and George Biros, University of Texas at Austin, USA

Monday, February 27

MS29

Measure Transport Approaches for Statistical Problems-Part I of II

10:15 AM-11:55 AM

Room:222

For Part 2 see MS58

Statistical problems such as parameter inference, data assimilation, and density estimation are ubiquitous in science and engineering. Solving these problems efficiently, however, becomes challenging with complicated datasets or nonlinear models. Recent years have seen considerable interest in tackling these problems via techniques based on nonlinear measure transformations. These transformations can be defined explicitly (e.g., via optimal transportation, Gaussianization) or implicitly via optimization (e.g., implicit filtering, randomize-then-optimize) or via the flows of ODEs. This minisymposium aims to explore connections among these measure transformation techniques and to provide a comprehensive view of their use in statistical inference and machine learning.

Organizer: Matthew Parno
US Army Cold Regions Research and Engineering Lab (CRREL), USA

Organizer: Alessio Spantini
Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk
Massachusetts Institute of Technology, USA

Organizer: Daniele Bigoni
Massachusetts Institute of Technology, USA

10:15-10:35 Bayesian Filtering and Smoothing Via Measure Transport

Alessio Spantini, Daniele Bigoni, and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

continued in next column

10:40-11:00 Discrete Monge-Kantorovich Approach for Large-Scale PDE-Constrained Bayesian Inverse Problems

Aaron Myers, University of Texas at Austin, USA

11:05-11:25 Flow Transport for Bayesian Inference

Jeremy Heng, University of Oxford, United Kingdom

11:30-11:50 Warp Bridge Sampling for Faster MCMC and for Multi-Modal Distributions

XiaoLi Meng, Harvard University, USA

Monday, February 27

CP1

Numerical Linear Algebra - Part I of III

10:15 AM-11:55 AM

Room:223

For Part 2 see CP3

Chair: To Be Determined

10:15-10:25 Theories and Algorithms of Integrated Singular Value Decomposition (iSVD)

Ting-Li Chen, Academia Sinica, Taiwan; D*awei D. Chang*, National Taiwan University, Taiwan; Su-Yun Huang, Academia Sinica, Taiwan; Hung Chen, National Taiwan University, Taiwan; Chienyao Lin, Academia Sinica, Taiwan; Weichung Wang, National Taiwan University, Taiwan

10:27-10:37 Parallel Implementations of Integrated Singular Value Decomposition (iSVD)

Mu Yang, National Taiwan University, Taiwan; Su-Yun Huang and Ting-Li Chen, Academia Sinica, Taiwan; Weichung Wang, National Taiwan University, Taiwan

10:39-10:49 Linear Equations and Eigenvalues Using Krylov Methods on Multiple Grid Levels

Ronald Morgan, Baylor University, USA

10:51-11:01 Polynomial Preconditioned Arnoldi for Eigenvalues

Jennifer A. Loe and Ronald Morgan, Baylor University, USA

11:03-11:13 Preconditioning Irk Methods for Time-Dependent Fluid Flow Problems

Victoria Howle, Texas Tech University, USA

11:15-11:25 A Fast Direct Solver for Elliptic PDEs on Locally-Perturbed Domains

Yabin Zhang and Adrianna Gillman, Rice University, USA

11:27-11:37 A Factored ADI Method for Sylvester Equations with High Rank Right Hand Sides

Heather D. Wilber, Boise State University, USA; Alex Townsend, Cornell University, USA

11:39-11:49 An Efficient Iterative Penalization Method Based on Recycled Krylov Subspaces and Its Application to Impulsively Started Flows

Thomas Gillis, Universite Catholique de Louvain, Belgium

Monday, February 27

CP2

Computational Fluid Dynamics - Part I of III

10:15 AM-11:55 AM

Room:224

For Part 2 see CP4

Chair: Brian Weston, University of California, Davis and Lawrence Livermore National Laboratory, USA

10:15-10:25 Physics-Based Preconditioning for a High-Order Rdg-Based Compressible Flow Solver with Phase Change

Brian Weston, University of California, Davis and Lawrence Livermore National Laboratory, USA; Robert Nourgaliev, Lawrence Livermore National Laboratory, USA; Jean-Pierre Delplanque, University of California, Davis, USA

10:27-10:37 Hierarchical Model Reduction for Incompressible Flows in Pipes

Sofia Guzzetti and Alessandro Veneziani, Emory University, USA; Simona Perotto, Politecnico di Milano, Italy

10:39-10:49 Inertial Confinement Fusion Simulations Using a Front Tracking API

Jeremy A. Melvin, Institute for Computational Engineering and Sciences, USA; Verinder Rana, Ryan Kaufman, and James Glimm, State University of New York, Stony Brook, USA

10:51-11:01 Stability of Oscillatory Rotating Boundary Layers

Scott N. Morgan, Cardiff University, United Kingdom

11:03-11:13 Conservative DEC Discretization of Incompressible Navier-Stokes Equations on Arbitrary Surface Simplicial Meshes With Applications

Mamdouh S. Mohamed, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Anil Hirani, University of Illinois at Urbana-Champaign, USA; Ravi Samtaney, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

continued in next column

11:15-11:25 Direct Computations of Marangoni-Induced Flows Using a Volume of Fluid Method

Ivana Seric, Shahriar Afkhami, and Lou Kondic, New Jersey Institute of Technology, USA

11:27-11:37 Marker Re-Distancing and Sharp Reconstruction for High-Order Multi-Material Front Dynamics

Robert Nourgaliev, Patrick Greene, and Sam Schofield, Lawrence Livermore National Laboratory, USA

Lunch Break

11:55 AM-1:30 PM

Attendees on their own

Monday, February 27

PD1

Student Careers Panel

12:15 PM-1:30 PM

Room:Ballroom D - 2nd Fl

Chair: Rebecca Li, Inria, France

Chair: Suzanne M. Shontz, University of Kansas, USA

The panelists will present an overview of careers in CSE in Academia, Industry and National Laboratories. The session will begin with brief presentations by the panelists, followed by an open discussion and question period with students in the audience. Lunch will be provided. Attendance is limited to current undergraduate and graduate students.

Michael Heroux
Sandia National Laboratories, USA

David Keyes
KAUST, Saudia Arabia and Columbia University, USA

Misha Kilmer
Tufts University, USA

Robert Schreiber
Hewlett-Packard Enterprise, USA

Monday, February 27

IP2

Challenges for Climate and Weather Prediction in the Era of Exascale Computer Architectures: Oscillatory Stiffness, Time-Parallelism, and the Role of Long-Time Dynamics

1:30 PM-2:15 PM

Room:Grand Ballroom - 2nd FL

Chair: Jan S. Hesthaven, École Polytechnique Fédérale de Lausanne, Switzerland

For weather or climate models to achieve exascale performance on next-generation heterogeneous computer architectures they will be required to exploit on the order of hundred-million-way parallelism. This degree of parallelism far exceeds anything possible in today's models even though they are highly optimized. In this talk I will discuss one of the mathematical issues that leads to the limitations in space- and time-parallelism for climate and weather prediction models – oscillatory stiffness in the PDE of the form: $\partial u/\partial t + 1/\varepsilon\, L(u) + N(u,u)=D(u)$, $u(0)=u_0$, where the linear operator L has pure imaginary eigenvalues, the quadratic nonlinear term is $N(u,u)$ D represents dissipation. The ε is a small non-dimensional parameter. The operator $\varepsilon^{-1}L$ results in time oscillations on an order $\mathcal{O}(\varepsilon)$ time scale, and generally requires small time steps for explicit methods, and implicit methods if accuracy is required. I will discuss the case when ε is finite and two algorithms: 1) a fast-converging HMM-parareal-type method and 2) a time-parallel matrix exponential.

Beth Wingate

University of Exeter, United Kingdom

Monday, February 27

Intermission

2:15 PM-2:25 PM

MT2

Version Control with Git-Part II

2:25 PM-4:05 PM

Room:Ballroom C - 2nd Fl

For Part 1 see MT1

Chair: Randall LeVeque, University of Washington, USA

The Git version control system is now widely used in the scientific computing community, not only for developing code (individually or collaboratively) but also for writing papers and grant proposals, sharing course materials with students and supporting group projects, and a host of other uses. The first part of this tutorial will introduce the basic concepts of Git and show how easy it is to get started using version control for your own work, on your own computer, as a good way to back up your work, keep track of changes you've made, revert to an earlier version if needed, and improve your ability to reproduce your own earlier work. The second part will cover more advanced concepts that are useful when using Git to collaborate with others, either privately or as part of an open source software community. We will cover branching, merging, forking, and the use of pull requests. We will also explore the tools available on GitHub, a popular collaboration site that hosts many open source projects. It is recommended that participants first install Git on their own laptops (see https://git-scm.com/book/en/v2/Getting-Started-Installing-Git) and create a free account on GitHub (see https://github.com/).

Randall LeVeque, University of Washington, USA; David I. Ketcheson, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Kyle T. Mandli, Columbia University, USA; Chris Vogl, University of Washington, USA

Monday, February 27

MS30

Career Fair: Careers in Business, Industry and Government - Part II of III

2:25 PM-4:05 PM

Room:Galleria

For Part 1 see MS1
For Part 3 see MS59

The career fair will feature employers from business, industry and government. These representatives will be prepared to discuss with you the opportunities for internships, postdoctoral appointments and full-time jobs at their organizations.

Organizer: William G. Kolata
SIAM, USA

Organizer: Kristin O'Neill
SIAM, USA

The Most Current List of Participating Companies Is Available at
http://www.siam.org/meetings/cse17/career.php

Monday, February 27

MS31

Inverse Problems Meet Big Data - Part II of III

2:25 PM-4:05 PM

Room:Grand Ballroom - 2nd Fl

For Part 1 see MS2
For Part 3 see MS60

Inverse and big-data problems are pervasive in engineering and science. Though in past decades tremendous advances in both theories and computational algorithms for inverse problems have been made, addressing big-data issue is less common. Larger datasets implies more memory/time in processing/storing/loading. Since the amount of data we wish to process is only going to increase for the foreseeable future, there is a critical need for inverse algorithms, such as data fitting methods, that are computation- and data-scalable. This minisymposium aims to engage researchers from inverse problems and big data problems in discussions about central questions of big data inverse problems.

Organizer: Matthias Chung
Virginia Tech, USA

Organizer: Tan Bui
University of Texas at Austin, USA

Organizer: Farbod Roosta-Khorasani
University of California, Berkeley, USA

2:25-2:45 Subspace Driven Data Reduction Strategies for Linear Bayesian Inverse Problems

Jayanth Jagalur Mohan and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

2:50-3:10 Faster Kernel Ridge Regression Using Sketching and Preconditioning

Haim Avron, Tel Aviv University, Israel

3:15-3:35 Randomized Matrix-Free Trace and Log-Determinant Estimators

Ilse Ipsen and Arvind Saibaba, North Carolina State University, USA; Alen Alexanderian, University of Texas at Austin, USA

3:40-4:00 Generalized Hybrid Iterative Methods for Large-Scale Bayesian Inverse Problems

Julianne Chung, Virginia Tech, USA; Arvind Saibaba, North Carolina State University, USA

Monday, February 27

MS32

Recent Advances in Local, Adaptive, and Multilevel Uncertainty Quantification Methods for Large-Scale Scientific Computing - Part II of III

2:25 PM-4:05 PM

Room:Ballroom D - 2nd Fl

For Part 1 see MS3
For Part 3 see MS61

Uncertainty quantification methods have seen tremendous use throughout the computational science community for enabling rigorous predictive simulation. In this minisymposium, recent advances in uncertainty quantification methods will be presented, focusing on local and adaptive methods applicable to problems involving localized behavior or discontinuities; multilevel methods exploiting hierarchies of fidelities for improved performance; and methods adapted for large-scale problems implemented on emerging extreme scale computer architectures.

Organizer: Eric Phipps
Sandia National Laboratories, USA

Organizer: Mohamed S. Ebeida
Sandia National Laboratories, USA

Organizer: Francesco Rizzi
Sandia National Laboratories, USA

2:25-2:45 Techniques for Reducing Computational Complexity of Sparse Grid Stochastic Collocation Methods

Peter Jantsch, University of Tennessee, USA; Clayton G. Webster, Oak Ridge National Laboratory, USA

2:50-3:10 Ensemble Grouping Strategies for Embedded Stochastic Collocation Methods

Marta D'Elia, Mohamed S. Ebeida, and Eric Phipps, Sandia National Laboratories, USA; Ahmad A. Rushdi, University of California, Davis, USA

continued in next column

3:15-3:35 An Ensemble Grouping Framework Based on Voronoi Piecewise Surrogate Models

Ahmad A. Rushdi, University of California, Davis, USA; Mohamed S. Ebeida, Marta D'Elia, and Eric Phipps, Sandia National Laboratories, USA

3:40-4:00 Computing Gradients in Local, Adaptive Voronoi Piecewise Surrogates

Eric Phipps, Marta D'Elia, Mohamed S. Ebeida, and H. Carter Edwards, Sandia National Laboratories, USA; Ahmad A. Rushdi, University of California, Davis, USA

Monday, February 27

MS33

Sparse Least Squares

2:25 PM-4:05 PM

Room:202

Linear least squares have had interesting applications since Gauss predicted the orbit of an asteroid in the early 1800s. For example, nonlinear least squares are typically solved through a sequence of linear least squares problems. Solving sparse problems allows scaling to large systems. We'll explore the interplay between iterative methods such as lsmr and lsqr and direct sparse factorization preconditioning. Talks will address both overdetermined and undetermined systems of equations.

Organizer: Gary W. Howell

North Carolina State University, USA

Organizer: Marc Baboulin

University of Paris-Sud, France

2:25-2:45 Using LU Factorization to Accelerate Convergence of Iterative Least Squares Solvers

Gary W. Howell, North Carolina State University, USA; Marc Baboulin, University of Paris-Sud, France

2:50-3:10 LU Preconditioning for Singular Sparse Least Squares

Michael A. Saunders, Stanford University, USA; Jennifer Scott and Nick Gould, Rutherford Appleton Laboratory, United Kingdom

3:15-3:35 Inner-Iteration Preconditioning for the Minimum-Norm Solutions to Least Squares Problem

Keiichi Morikuni, University of Tsukuba, Japan

3:40-4:00 Preconditioning Linear Least-Squares Problems by Identifying a Basis Matrix

Mario Arioli, Université Toulouse I, France; Iain Duff, Science & Technology Facilities Council, United Kingdom and CERFACS, Toulouse, France

Monday, February 27

MS34

Extreme Scale Solvers - Part II of II

2:25 PM-3:40 PM

Room:203

For Part 1 see MS5

Exascale computers will exhibit billion-way parallelism. Computing on such extreme scale needs methods scaling perfectly with optimal complexity. This minisymposium combines talks on crucial aspects of extreme scale solving. The solver must be of optimal complexity, which is more an more severe with increasing problem size, and scale efficiently on extreme scales of parallelism. To that end, the minisymposium brings together talks on parallel adaptive multigrid methods in space and time, on nonlinear domain decomposition methods, as well as optimziation and uncertainty quantification techniques. Also, industrial applications and software aspects will be considered.

Organizer: Rolf Krause

Università della Svizzera italiana, Switzerland

Organizer: Gabriel Wittum

King Abdullah University of Science & Technology (KAUST), Saudi Arabia

2:25-2:45 Exascale Solvers in UG - Multigrid for HPC

Gabriel Wittum, University of Frankfurt, Germany

2:50-3:10 Nonlinear Domain Decomposition Methods for Large Scale Problems

Rolf Krause, Università della Svizzera italiana, Switzerland

3:15-3:35 A New Iterative Scheme Based on DG Methods for (Parallel) Time Integration

Xiaozhou Li, *Pietro Benedusi*, and Rolf Krause, Università della Svizzera italiana, Switzerland

Monday, February 27

MS35

Computational and Numerical Methods in Electronics - Part II of II

2:25 PM-4:05 PM

Room:204

For Part 1 see MS6

Research in electronics faces two challenges which are unfortunately often considered separate from each other: First, the rapid technological progress requires short simulation times for electronic devices with increasing geometric complexity. Such short simulation times can only be achieved through the development of new parallel algorithms since the serial performance of modern computing hardware stagnates. Second, sound numerical methods are required to accurately describe electronic transport at the discrete level. For example, important physical properties such as positivity and charge conservation need to be reflected in the numerics. This minisymposium aims at bridging the gap between both challenges by providing an interdisciplinary platform for physicists, numerical analysts and computational scientists.

Organizer: Karl Rupp

Freelance Computational Scientist, Austria

Organizer: Josef Weinbub

Christian Doppler Laboratory for High Performance TCAD, TU Wien, Austria

Organizer: Patricio Farrell

Weierstrass Institute, Germany

Organizer: Nella Rotundo

Weierstrass Institute, Germany

2:25-2:45 How Do Electrons Move in Space? Flux Discretizations for Non-Boltzmann Statistics

Patricio Farrell, Thomas Koprucki, and J. Fuhrmann, Weierstrass Institute, Germany

continued on next page

2:50-3:10 Numerical Algorithms Based on Galerkin Methods for the Modeling of Reactive Interfaces in Photoelectrochemical Solar Cells

Michael D. Harmon, Kui Ren, and Irene M. Gamba, University of Texas at Austin, USA

3:15-3:35 Modeling and Simulations Using Time-Dependent Density Functional Theory

James Kestyn and Eric Polizzi, University of Massachusetts, Amherst, USA

3:40-4:00 NEMO5: A Parallelized Multi-Scale and Multi-Physics Nanodevices Simulation Software

Xinchen Guo, Daniel Lemus, Daniel Mejia, Jim Fonseca, Gerhard Klimeck, and Tillmann Kubis, Purdue University, USA

Monday, February 27

MS36

Modeling and Computational Methods in Network Science and Applications - Part II of II

2:25 PM-3:40 PM

Room:205

For Part 1 see MS7

In recent years, there has been high demand for novel and accurate mathematical models, and fast, stable and scalable computational techniques to address problems emerging from applications on real-world networks, such as social media and power grids. In these applications, big data is often generated, collected, stored and/or processed in large-scale heterogeneous networks. New models and computational methods must tackle challenges of inhomogeneous structures of networks, randomness of dynamics, and noise in data. This minisymposium focuses on the recent advances of mathematical modeling and numerical methods as well as their applications in modern network science.

Organizer: Xiaojing Ye

Georgia State University, USA

Organizer: Honguyan Zha

Georgia Institute of Technology, USA

Organizer: Haomin Zhou

Georgia Institute of Technology, USA

2:25-2:45 Enhanced Community Detection in Multilayer and Temporal Networks through Layer Aggregation

Dane Taylor, University of North Carolina at Chapel Hill, USA; Rajmonda Caceres, Massachusetts Institute of Technology, USA; Peter J. Mucha, University of North Carolina at Chapel Hill, USA

2:50-3:10 Real-Time In-Situ Seismic Imaging with Sensor Networks

WenZhan Song, University of Georgia, USA

3:15-3:35 Abnormal Synchrony in Evolving Brain Networks

Igor Belykh, Reimbay Reimbayev, and Kevin Daley, Georgia State University, USA

Monday, February 27

MS37

Smooth, Reduced, Sparse -- Exploiting Structures for Surrogate Modeling in CSE- Part II of III

2:25 PM-4:05 PM

Room:206

For Part 1 see MS8
For Part 3 see MS66

This minisymposium explores and highlights techniques that exploit structures in computationally expensive high-fidelity models to derive accurate low-cost surrogate models. A prominent example is projection-based model reduction, which exploits that states of the high-fidelity model can be approximated well in a reduced space of low dimension. Other methods exploit the smoothness of functions that are induced by the high-fidelity model (e.g., input-output and parameter-output maps), or sparsity of representations of the high-fidelity model outputs in well-chosen bases.

Organizer: Benjamin Peherstorfer

Massachusetts Institute of Technology, USA

Organizer: Gianluigi Rozza

SISSA-ISAS International School for Advanced Studies, Italy

2:25-2:45 About Empirical Interpolation Methods and Applications

Yvon Maday, Université Pierre et Marie Curie, France

2:50-3:10 Error Control As a Key Ingredient Towards Optimal Numerical Methods

Mario Ohlberger, Stephan Rave, and Felix Schindler, Universität Münster, Germany

3:15-3:35 Non-Smoothness in Space and Time Within Model Reduction

Silke Glas and Karsten Urban, University of Ulm, Germany

3:40-4:00 Certified Reduced Basis Methods for 4D-Var Data Assimilation

Karen Veroy-Grepl, Martin Grepl, and Mark Kaercher, RWTH Aachen University, Germany

Monday, February 27

MS38

Hierarchically Rank-Structured Matrix Techniques - Part II of II

2:25 PM-4:05 PM

Room:209

For Part 1 see MS9

Rank-structured methods have demonstrated significant advantages in improving the efficiency and reliability of some large-scale computations and engineering simulations. These methods extend the fundamental ideas of multipole and panel-clustering methods to general non-local solution operators. While there exist various more or less closely related methods, the unifying aim of these methods is to explore efficient structured low-rank approximations, especially those exhibiting hierarchical or nested forms. In this minisymposium, we aim to present and exchange recent new developments such as efficient linear complexity algorithms, the construction of direct solvers for partial differential and integral equations, structured eigenvalue solutions, structured preconditioning, randomized algorithms, as well as implementation aspects.

Organizer: Sabine Le Borne

Hamburg University of Technology, Germany

Organizer: Jianlin Xia

Purdue University, USA

2:25-2:45 Fast Low-Rank Approximation of a Matrix and Extensions

Victor Pan, City University of New York, USA

2:50-3:10 Effective and Robust Preconditioning of General SPD Matrices with Rank Structures

Jianlin Xia and Zixing Xin, Purdue University, USA

continued in next column

3:15-3:35 Compute-Memory Tradeoff in Hierarchical Low-Rank Approximation Methods

Rio Yokota, Tokyo Institute of Technology, Japan; David E. Keyes, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

3:40-4:00 A Fast Contour-Integral Eigensolver and the Approximation Accuracy

Xin Ye and Jianlin Xia, Purdue University, USA; Raymond H. Chan, Chinese University of Hong Kong, Hong Kong

Monday, February 27

MS39

Monte Carlo and Ensemble Methods for Uncertainty Quantification

2:25 PM-4:05 PM

Room:210

For Part 1 see MS10

A common goal of uncertainty quantification is the calculation of probabilities, expected values, etc. of a random variable. Given a probability density function these quantities can be represented as integrals. Monte Carlo integration is frequently used to compute multidimensional integrals due to its dimensionally independent convergence. However, this convergence is often slow which is troublesome when the random variable involved is obtained from an expensive computational model or the event has complicated geometry. This minisymposium explores techniques for efficiently sampling stochastic space to compute multidimensional integrals with emphasis on ensemble model evaluations, efficient use of multifidelity models, and sample selection.

Organizer: Lindley C. Graham

Florida State University, USA

Organizer: Nan Jiang

Missouri University of Science and Technology, USA

2:25-2:45 The Multi-Level Monte Carlo Method for Simulations of Turbulent Flows

Qingshan Chen, Clemson University, USA; Ming Ju, Beijing Computational Science Research Center, China

2:50-3:10 Multifidelity Monte Carlo Methods with Optimally-Adapted Surrogate Models

Benjamin Peherstorfer and Karen E. Willcox, Massachusetts Institute of Technology, USA

3:15-3:35 Acceleration of the Multilevel Monte Carlo Method for Certain Classes of Differential Systems

Viktor Reshniak, Abdul Khaliq, and Yuri Melnikov, Middle Tennessee State University, USA

3:40-4:00 Reduced Basis Methods and Their Application to Ensemble Methods for the Navier Stokes Equations

Michael Schneier, Florida State University, USA

Monday, February 27

MS40

Integral Equation Methods for Particulate Flows - Part II of II

2:25 PM-4:05 PM

Room:211

For Part 1 see MS11

This minisymposium will focus on recent advances in the development and/or application of integral equation methods for low-Re viscous flow of drops, vesicles, rigid particles or other particulate suspensions.

Organizer: Shravan Veerapaneni

University of Michigan, USA

2:25-2:45 Hydrodynamic and Macromolecules Induced Clusters of Red Blood Cells in Microcapillary Flow

Chaouqi Misbah, Universite Joseph Fourier, France

2:50-3:10 Calculation of Apparent Viscosity Using Boundary Integral Equations

Lukas Bystricky and Bryan D. Quaife, Florida State University, USA

3:15-3:35 A Second-Kind Traction Integral Equation for Wall-Bounded Viscous Flows, with Applications to Sedimentation and Viscous Erosion

William Mitchell and Saverio E. Spagnolie, University of Wisconsin, USA

3:40-4:00 Global Stability of Fully Coupled Capsule Flow Systems

Spencer H. Bryngelson and Jonathan B. Freund, University of Illinois at Urbana-Champaign, USA

Monday, February 27

MS41

Multifidelity Simulation and Approximation in the Computational Sciences - Part I of II

2:25 PM-4:05 PM

Room:212

For Part 2 see MS70

A modern computational mainstay is the multifidelity challenge: make efficient and robust predictions given several competing models each having its own degree of trust. The abstract concept of "fidelity" -- faithfulness to physics, experimental observations, and/or idealized mathematical formulations -- arises because different simulation suites utliize different discretization types and scales, and make dissimilar simplifications of underlying physics. This minisymposium aims to highlight recent advances in algorithms that make optimal use of models with differing fidelities. The challenges include resource distribution among models, identification and learning of model hierarchy, and efficient synthesis of model predictions.

Organizer: Akil Narayan

University of Utah, USA

Organizer: Xueyu Zhu

University of Iowa, USA

2:25-2:45 Stochastic Collocation with Multi-Fidelity Models

Xueyu Zhu, University of Iowa, USA; Akil Narayan and Linebarger Erin, University of Utah, USA; Dongbin Xiu, Ohio State University, USA

2:50-3:10 A Bi-Fidelity, Low-Rank Approximation Technique for Uncertainty Quantification

Hillary Fairbanks, Jerrad Hampton, and Alireza Doostan, University of Colorado Boulder, USA; Akil Narayan, University of Utah, USA

3:15-3:35 Multifidelity Monte Carlo Methods for Uncertainty Quantification

Karen E. Willcox and Benjamin Peherstorfer, Massachusetts Institute of Technology, USA

3:40-4:00 Prediction Based on the Kennedy-O'Hagan Calibration Model: Asymptotic Consistency and Other Properties

Rui Tuo, Chinese Academy of Sciences, China; Jeff Wu, Georgia Institute of Technology, USA

Monday, February 27

MS42

Recent Advance on Numerical Methods for Quantum Problems - Part II of III

2:25 PM-4:05 PM

Room:213

For Part 1 see MS13
For Part 3 see MS71

Quantum problems have numerous applications in quantum physics and chemistry, plasma and particle physics, material sciences, semiconductor theory, rarefied gas theory, Bose-Einstein condensation, nonlinear optics, erc. The typical models include nonlinear Schroedinger equation (NLS), Dirac equation, Klein-Gordon equation, density fucntional theory, quantum Boltzmann equation, etc. The purpose of this minisymposium is to provide a platform for the researchers in the field to present recent work on the numerical analysis, numerical methods and simulation for these quantum problems, to exchange idea and to discuss future directions in the field.

Organizer: Yongyong Cai

Beijing Computational Science Research Center, China

2:25-2:45 High-Order Numerical Schemes for Computing the Dynamics of Nonlinear Schrödinger Equation

Christophe Besse, University of Toulouse III, France

2:50-3:10 Accelerated Gradient Methods for Computing the Stationary States of Gross-Pitaevskii Equations

Xavier L. Antoine and Qinglin Tang, Université de Lorraine, France; Antoine Levitt, Inria and Ecole des Ponts ParisTech, France

3:15-3:35 Efficient Spectral Methods for Electronic Schrodinger Equation

Yingwei Wang and Jie Shen, Purdue University, USA; Haijun Yu, Institute of Computational Mathematics, China

3:40-4:00 Accurate and Efficient Computation of Nonlocal Potentials Based on Gaussian-Sum Approximation

Yong Zhang, Wolfgang Pauli Institute, Austria

Monday, February 27

MS43

Neutrino Transport Methods in Astrophysics

2:25 PM-4:05 PM

Room:214

For Part 1 see MS14

Core-collapse supernovae (CCSNe) and neutron star mergers are cataclysmic astrophysical events responsible for heavy element synthesis and the emission of photon, neutrino, and gravitational wave signals. They have long been targets of instruments covering most of the electromagnetic spectrum, and more recently of neutrino and gravitational wave detectors (e.g. IceCube and LIGO). Harvesting insights into the physical processes driving these events from this wealth of data relies heavily on sophisticated models requiring extreme-scale, high-fidelity computing. These models solve a coupled system of equations for self-gravity, magneto-hydrodynamics, and neutrino transport. For example, about 99% of the gravitational energy released during a CCSN is radiated away in the form of neutrinos, which are likely a major driver of the supernova explosion. However, neutrino-matter interactions occur under non-equilibrium conditions (neutrinos are semi-transparent to the stellar fluid) and a description based on the Boltzmann transport equation is warranted. As a six-dimensional phase-space problem, our ability to model these astrophysical events with satisfactory realism relies on advances in multi-physics and multi-scale algorithms, novel discretization techniques, fast solvers, and sustainable scientific software. The goal of this minisymposium is to bring together researchers working on topics of relevance to neutrino transport modeling to discuss recent work and exchange ideas.

continued in next column

Organizer: Eirik Endeve
Oak Ridge National Laboratory, USA

Organizer: Reuben Budiardja
University of Tennessee, USA

2:25-2:45 Neutrino Transport in Neutron Star Merger Simulations

Francois V. Foucart, Lawrence Berkeley National Laboratory, USA

2:50-3:10 Neutrino Radiation-Hydrodynamics Simulations of Neutron Star Mergers

David Radice, Princeton University, USA

3:15-3:35 Neutrino Transport in Core Collapse Supernovae

Luke Roberts, Michigan State University, USA

3:40-4:00 Discontinuous Galerkin Methods for Neutrino Radiation-Hydrodynamics

Eirik Endeve, Oak Ridge National Laboratory, USA; Anthony Mezzacappa, University of Tennessee, USA

Monday, February 27

MS44

Efficiency of High-Order Methods on the 2nd Generation Intel Xeon Phi Processor - Part II of II

2:25 PM-4:05 PM

Room:215

For Part 1 see MS15

In Summer 2016 the 2nd generation Intel Xeon Phi Processor (Knights Landing) was released. It will be the computational heart of many future supercomputing installations. Examples are the DoE-machines "Trinity-II", "Cori-II" and "Theta", "Stampede-2" of NSF, or the future 25 PFLOPS machine "Oakforest-PACS" in Japan. The 2nd generation of the Xeon Phi processor combines the computational power of accelerator-based machines with the traditional approach of homogeneous high performance computing. From an application viewpoint, many research articles in the last years have proven that high-order methods require the computational power of modern supercomputers. However, it is a challenging engineering problem to enable complex software packages on manycore architectures. This minisymposia brings together researchers working on efficient implementations of scalable higher-order solvers. Of particular interest are applications which are known to require exascale computing resources in future, such as computational fluid dynamics, electro-magnetics and seismic simulations, as well as weather forecasting. Due to the broad spectrum of applications, this MS aims at identifying common algorithmic patterns of efficient high-order methods. Additionally, the comparison of different numerical approaches (e.g. CG vs. DG) will allow to identify best practices and an early performance/ease-of-use estimator when leveraging Intel Xeon Phi systems at scale.

Organizer: Alexander Heinecke
Intel Corporation, USA

continued on next page

Organizer: Alexander Breuer
University of California, San Diego, USA

2:25-2:45 Performance Optimizations for the SU2 Higher-Order DG-FEM Fluid Solver on the Intel Xeon Phi
Edwin van der Weide, University of Twente, Netherlands; *Juan J. Alonso* and Thomas Economon, Stanford University, USA

2:50-3:10 Large-Scale Dynamic Rupture Simulations with SeisSol on KNL Platforms
Carsten Uphoff, Sebastian Rettenberger, Michael Bader, and Alice Gabriel, Technische Universität München, Germany

3:15-3:35 Vectorization and Locality Optimizations for Seismic Imagining Methods Through Automated Code Generation
Fabio Luporini, Gerard J Gorman, Paul Kelly, and Michael Lange, Imperial College London, United Kingdom

3:40-4:00 Performance of the Non-Hydrostatic Unified Model of the Atmosphere on the Intel Knights Landing
Daniel Abdi, Francis X. Giraldo, and Lucas Wilcox, Naval Postgraduate School, USA; Tim Warburton, Virginia Tech, USA; David Medina, Rice University, USA; Andreas Mueller, Naval Postgraduate School, USA

Monday, February 27

MS45

Automatic Code Generation for Simulation and Optimization - Part II of II

2:25 PM-4:05 PM

Room:216

For Part 1 see MS16

Scientific computing plays an ever increasing role in understanding complex physical processes and computer simulations are nowadays an indispensable tool in many fields and applications. Recent trends with respect to creating and maintaining high fidelity simulation codes for partial differential equations governing such problems are high level languages and automatic code generation. Being able to postulate a problem in a programming paradigm, which is both close to the mathematical problem description and can be processed by a computer, naturally makes understanding, developing and maintaining complex codes much easier. Transitioning to solving optimization problems is the next natural step. With the advent of high level domain specific programming languages such as UFL, it only nowadays becomes feasible to create unified code generation approaches for the primal and adjoint problem, where the differentiation tool has information available about the nature of the primal problem and the meaning of the instructions and variables it is currently processing, thereby creating a hybridized optimization framework between the continuous and discrete approach automatically. With these developments in mind, the aim of this minisymposium is to bring together the various recent trends in code generation for simulation and optimization with the intention to foster new structure exploiting hybridization strategies.

Organizer: Stephan Schmidt
Universität Würzburg, Germany

Organizer: Nicolas R. Gauger
Technische Universität Kaiserslautern, Germany

continued in next column

2:25-2:45 Automatic Adjoints of Multimesh Finite Element Discretisations
Simon W. Funke, Jørgen Dokken, and August Johannson, Simula Research Laboratory, Norway

2:50-3:10 Algorithmic Differentiation of a CAD System for Shape Optimization
Andrea Walther, Universität Paderborn, Germany

3:15-3:35 Automating Optimal Code Generation for High Order Finite Element Methods
David Ham, Imperial College, United Kingdom

3:40-4:00 Exporting ADOL-C API for Scripting Languages Using SWIG
Kshitij Kulshreshtha, Universität Paderborn, Germany; Sri Hari Krishn Narayanan, Argonne National Laboratory, USA

Monday, February 27

MS46

Advances in MCMC and Related Sampling Methods for Large-Scale Inverse Problems - Part II of II

2:25 PM-4:05 PM

Room:217

For Part 1 see MS17

Inverse problems convert indirect measurements into useful characterizations of the parameters of a physical system. Parameters are typically related to indirect measurements by a system of partial differential equations (PDEs), which are complicated and expensive to evaluate. Available indirect data are often limited, noisy, and subject to natural variation, while the unknown parameters of interest are often high dimensional, or infinite dimensional in principle. Solution of the inverse problem, along with prediction and uncertainty assessment, can be cast in a Bayesian setting and thus naturally tackled with Markov chain Monte Carlo (MCMC) and other posterior sampling methods. However, designing scalable and efficient sampling methods for high dimensional inverse problems that involve expensive PDE evaluations poses a significant challenge. This minisymposium presents recent advances in sampling approaches for large scale inverse problems.

Organizer: Tiangang Cui

Monash University, Australia

Organizer: Youssef M. Marzouk

Massachusetts Institute of Technology, USA

Organizer: Tan Bui-Thanh

University of Texas at Austin, USA

2:25-2:45 A Gaussian Process Prior Approach to Estimating Parameters in Multi-level Stochastic Differential Equations

Peter Craigmile and R*adu Herbei*, Ohio State University, USA

2:50-3:10 Fast Experimental Designs for LARGE Linear Processes: How to Image Biofilms Using a 3-D Confocal Scanning Laser Microscope

Albert E. Parker, Montana State University, USA

3:15-3:35 Regularized Estimation of Likelihood-Informed Subspaces from Samples

Olivier Zahm and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

3:40-4:00 Marginal then Conditional Sampling for Hierarchical Models

Colin Fox and Richard A. Norton, University of Otago, New Zealand; J. Andrés Christen, Centro de Investigacion en Matematicas, Mexico

continued in next column

Monday, February 27

MS47

Algorithms and Libraries for Tensor Contractions - Part II of II

2:25 PM-4:05 PM

Room:218

For Part 1 see MS18

Tensors and tensor contractions are the multi-dimensional generalization of matrices and matrix products, respectively. They arise in a multitude of disciplines and applications, ranging from theoretical physics to quantum chemistry and machine learning. Interestingly, while the performance of the kernels for matrix-products (GEMM) is typically excellent, that of tensor contractions is often far from optimal. The difference is due to a number of factors, including the sheer size of the tensors, the suboptimal memory access patterns, the increased complexity to achieve locality, and possibly a low arithmetic intensity. This minisymposium is devoted to algorithms and libraries for the efficient calculation of tensor contractions. The existing approaches can be loosely classified in three categories: nested-loops, transpose-transpose-GEMM-transpose, and loops-over-GEMMs. With these eight talks, we bring together experts from all three categories, presenting a thorough overview of the state of the art in the field of high-performance tensor contractions.

Organizer: Paolo Bientinesi

RWTH Aachen University, Germany

2:25-2:45 A Distributed Memory Library for Sparse Tensor Functions and Contractions

Edgar Solomonik, University of Illinois at Urbana-Champaign, USA

2:50-3:10 Strongly-Scalable Block and Rank-Sparse Tensor Algebra

Edward F. Valeev, Virginia Tech, USA

continued on next page

3:15-3:35 Accelerating Tensor Contractions by Runtime Code Generation of Small Matrix Multiplications on Intel Architecture

Alexander Heinecke, Greg Henry, and Hans Pabst, Intel Corporation, USA

3:40-4:00 Accelerating Tensor Contractions in High-Order FEM with MAGMA Batched

Stanimire Tomov, University of Tennessee, Knoxville, USA; Azzam Haidar, University of Tennessee, USA; Ahmad Abdelfattah, University of Tennessee, Knoxville, USA; Veselin Dobrev, Ian Karlin, and Tzanio V. Kolev, Lawrence Livermore National Laboratory, USA; Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA

Monday, February 27

MS48

Applications and Computational Strategies for Finite Element Computations using LibMesh - Part II of II

2:25 PM-4:05 PM

Room:219

For Part 1 see MS19

The development of the libMesh finite element library began over a decade ago in order to support adaptive mesh refinement on unstructured grids for finite element simulations of complex applications. It has grown to support hundreds of users across the world, has been used and scaled on large parallel supercomputers, and enabled the study of a wide variety of finite element computations. This minisymposium aims to bring together users and developers of the libMesh finite element library to discuss the latest developments in the library, frameworks supported by the libMesh, and applications enabled by the libMesh infrastructure.

Organizer: Paul Bauman
State University of New York at Buffalo, USA

Organizer: Alvaro Coutinho
Federal University of Rio de Janerio, Brazil

Organizer: John W. Peterson
Idaho National Laboratory, USA

Organizer: Roy Stogner
University of Texas at Austin, USA

2:25-2:45 An Overview of the Moose Framework and Physics Modules

John W. Peterson, Derek R. Gaston, Cody J. Permann, David Andrs, Andrew Slaughter, and Brian Alger, Idaho National Laboratory, USA; Fande Kong, University of Colorado Boulder, USA; Richard Martineau, Idaho National Laboratory, USA

2:50-3:10 Rattlesnake: A Moose/libmesh-Based Multiscale Neutronics Application

Sebastian Schunert, Yaqi Wang, and Mark DeHart, Idaho National Laboratory, USA

continued in next column

3:15-3:35 An Overview of the GRINS Multiphysics Framework

Paul Bauman, State University of New York at Buffalo, USA

3:40-4:00 In Situ Data Steering with Provenance Data

Vitor Silva, José Camata, and Marta Mattoso, Federal University of Rio de Janerio, Brazil; Patrick Valduriez, Inria, France; *Alvaro Coutinho*, Federal University of Rio de Janerio, Brazil

Monday, February 27

MS49

Toward Resiliency via Numerical Remedies - Part II of II

2:25 PM-4:05 PM

Room:220

For Part 1 see MS20

Future extreme scale systems are expected to suffer more frequent hard faults and soft error resulting from the unprecedented scale of parallelism. Combined with the technology trend such as the imbalance between computing and I/O throughput and a tight power budget in the system operations, the traditional hardware-level redundancy and checkpoint restart may not be a feasible solution. Although, every layer of the systems should address these faults to mitigate their impact in holistic manners, we will focus in this minisymposium the deficiencies from a algorithm and applications viewpoint.

Organizer: Keita Teranishi

Sandia National Laboratories, USA

Organizer: Luc Giraud

Inria, France

Organizer: Emmanuel Agullo

Inria, France

Organizer: Michael Heroux

Sandia National Laboratories, USA

2:25-2:45 Soft Error in PCG: Sensitivity, Numerical Detections and Possible Recoveries

Emmanuel Agullo and Luc Giraud, Inria, France

2:50-3:10 Resilient Dense/Sparse Linear Algebra

Zizhong Chen, University of California, Riverside, USA

3:15-3:35 Programming Constructs for Transparent Silent-Error Mitigation in PDE Solvers

Maher Salloum, Jackson Mayo, and Rob Armstrong, Sandia National Laboratories, USA

3:40-4:00 Integrating Algorithm Based Fault Tolerance into a Parallel Mulitigrid Library

Brian Austin and Xiaoye S. Li, Lawrence Berkeley National Laboratory, USA

Monday, February 27

MS50

Scientific Workflow Environment toward Extreme-Scale Computing - Part II of II

2:25 PM-4:05 PM

Room:Crystal AF - 1st Fl

For Part 1 see MS21

The continuous progress in high performance and cloud computing technology has enabled scientists and engineers to understand multi-scale and multi-physics phenomena at unprecedented complexity and scale. Today, many science and engineering computations are comprised with multiple application programs including compute-intensive simulations, data analytics and visualization. For such application couplings, scientific workflow software is essential to express the interactions among these programs transparently and seamlessly connect them in platform independent manner. In addition to such couplings, the workflow provides a steerings to use to dynamically control program executions and input parameter settings to permit the users to investigate the point of their interest with a better focus. In this minisymposium, we discuss the techniques and challenges of scientific-workflow for future extreme scale computing environment, including performance, scalability, resilience, and usability issues.

Organizer: Keita Teranishi

Sandia National Laboratories, USA

Organizer: Martin Schulz

Lawrence Livermore National Laboratory, USA

continued in next column

2:25-2:45 HPC Workflow Taxonomies: A New Methodology for Hardware/ Software CoDesign

David Montoya, Los Alamos National Laboratory, USA

2:50-3:10 Engineering Sciences Workflows for V&V Applications

Robert Clay, Ernest Friedman-Hill, and Edward Hoffman, Sandia National Laboratories, USA

3:15-3:35 Workflow Modernization Efforts at Lawrence Livermore National Laboratory

Daniel Laney, Lawrence Livermore National Laboratory, USA

3:40-4:00 Swift: Implicitly Parallel Workflow for Science and Engineering Applications

Michael Wilde, Argonne National Laboratory, USA; Justin Wozniak, Argonne National Laboratory and University of Chicago, USA

Monday, February 27

MS51

Model Discrepancy and Model Form Error: Bayesian Approaches

2:25 PM-3:40 PM

Room:Crystal CD - 1st Fl

For Part 1 see MS22

Model discrepancy is defined as the difference between model predictions and experimental data, sometimes called "model form error" or "structural model error". There are a variety of approaches being developed, including formulations that represent discrepancy explicitly using, for example, Gaussian processes or polynomial chaos expansions, as well as implicit formulations in which "model correction" terms are determined concurrently with the solution of a set of partial differential equations. Approaches that are Bayesian or non-Bayesian in nature, along with those supported by machine learning principles, may be used to estimate model discrepancy. This minisymposium encompasses the Bayesian approaches and is meant to foster discussion of the various methods.

Organizer: Laura Swiler

Sandia National Laboratories, USA

Organizer: Kathryn Maupin

Sandia National Laboratories, USA

2:25-2:45 Model Discrepancy Formulations in Dakota

Kathryn Maupin and Laura Swiler, Sandia National Laboratories, USA

2:50-3:10 Bayesian Calibration of Engineering Hydraulic Fracturing Models in the Presence of Parametric Uncertainties and Model Errors

Fernando A. Rochinha, COPPE/Universidade Federal do Rio e Janeiro, Brazil; Souleymane Zio, Federal University of Rio de Janerio, Brazil

3:15-3:35 Bayesian Selection of Model-Model Connections in Multiscale Hierarchies with Uncertainty in Calibration

Aaron E. Tallman, Georgia Institute of Technology, USA; Laura Swiler, Sandia National Laboratories, USA; Yan Wang and David McDowell, Georgia Institute of Technology, USA

Monday, February 27

MS52

Stochastic PDE-Constrained Optimization and Applications - Part II of II

2:25 PM-4:05 PM

Room:301

For Part 1 see MS23

Engineering decisions are often formulated as optimization problems constrained by partial differential equations (PDEs). Unfortunately, these governing PDEs are typically fraught with uncertainties including input parameters estimated from noisy and incomplete data, unknown initial and boundary conditions, and unverifiable modeling assumptions. Thus, the need to make robust or risk-averse decisions pervades nearly all engineering applications including, e.g., optimal control and design, and inverse problems. Due to the array of computational and theoretical difficulties associated with these problems, it is critical to develop new techniques in stochastic programming, PDE-constrained optimization and tensor methods. The goal of this multi-part minisymposium is to showcase new research in these areas with application to PDE-constrained optimization under uncertainty.

Organizer: Drew P. Kouri

Sandia National Laboratories, USA

Organizer: Thomas M. Surowiec

Philipps-Universität Marburg, Germany

2:25-2:45 Risk Averse Optimization for Material Science

Bart G. Van Bloemen Waanders, Sandia National Laboratories, USA

2:50-3:10 Low-Rank Tensor Methods for Constrained Optimization Problems with PDEs under Uncertainty

Michael Ulbrich and Sebastian Garreis, Technische Universität München, Germany

3:15-3:35 Optimal Control of Fractional Power of Elliptic Operators

Harbir Antil, George Mason University, USA

3:40-4:00 An Adaptive Approach for Solving Stochastic Partial Differential Equations using Reduced Local Bases

Wilkins Aquino and Zilong Zhou, Duke University, USA

Monday, February 27

MS53

Advances in Enabling Quantification of Uncertainty in Physical Systems (EQUiPS)– Part II of II

2:25 PM-4:05 PM

Room:302

For Part 1 see MS24

Uncertainty quantification (UQ) is key for achieving validated predictive computations in a wide range of complex scientific and engineering applications. However, many fundamental challenges still remain in trying to build effective predictive models in engineering design of large, multi-physics and multi-scale physical systems. Existing computational and theoretical approaches and methodologies cannot adequately handle uncertainty emerging from high dimensional input parameter spaces, model form discrepancies, and random conditions in the operating environment of these systems. This minisymposium intends to explore and present advances at the forefront of research in these topics, ranging from highly efficient for both "forward" and "inverse" UQ algorithms to novel physics-based methodologies to capture model form uncertainty, leading to robust and dynamic decision-making frameworks for design under uncertainty. Topics include: Entropy metrics to measure model errors, multi-fidelity information fusion algorithms to quantify failure and rare events, new methods for likelihood estimation in Bayesian inference for inverse problems, and optimal control and design of turbulent flow systems under uncertainty.

Organizer: Fariba Fahroo

Air Force Office of Scientific Research, USA

continued on next page

Monday, February 27

MS53

Advances in Enabling Quantification of Uncertainty in Physical Systems (EQUiPS)–Part II of II

2:25 PM-4:05 PM

continued

2:25-2:45 Universal Scalable Robust Solvers from Computational Information Games

Houman Owhadi, and Clint Scovel, California Institute of Technology, USA

2:50-3:10 Adaptive Sampling for Risk-Averse PDE-Constrained Optimization

Drew P. Kouri, Sandia National Laboratories, USA

3:15-3:35 UQ Prediction Under Limited Resources

Dongbin Xiu, University of Utah, USA

3:40-4:00 Scalable Methods for Rare Event Simulation in Rotocraft Systems

Benjamin Zhang and Youssef M. Marzouk, Massachusetts Institute of Technology, USA; *Tuhin Sahai*, United Technologies Research Center, USA

Monday, February 27

MS54

Direct and Inverse Problems in Numerical Modeling of Cardiac Electrophysiology

2:25 PM-4:05 PM

Room:303

For Part 1 see MS25

Numerical cardiac electrophysiology has been developed for quantitatively understanding the dynamics of potential propagation in the heart. Notwithstanding the progressive refinement of models and methods, several challenges are still on. (1) The description of specific features (e.g. cardiac fibers) still requires modeling developments; (2) the patient specific perspective demands the efficient solution of inverse parameter estimation problems. This Minisymposium gathers mathematicians, physicists and engineers working on different sides of the problem for reliably solving both direct and inverse problems in electrophysiology. Modeling/computational aspects, uncertainty quantification, validation and the point of view of clinicians will be represented. Supported by NSF.

Organizer: Alessandro Veneziani

Emory University, USA

Organizer: Flavio H. Fenton

Georgia Institute of Technology, USA

2:25-2:45 Influence of Cardiac Mechano-Electric Feedback on Reentry Dynamics: A Simulation Study

Piero Colli Franzone, University of Pavia, Italy; *Luca F. Pavarino*, University of Milan, Italy; Simone Scacchi, Universita degli Studi di Milano, Italy; Stefano Zampini, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

2:50-3:10 Numerical Modeling of the Electrical Activity in the Ventricles in Presence of Detailed Purkinje Fibers

Christian Vergara, Politecnico di Milano, Italy

3:15-3:35 A Luenberger Observer for Reaction-Diffusion Models with Front Position Data

Annabelle Collin, Universite de Bordeaux I, France; Dominique Chapelle, Inria, France; Philippe Moireau, INRA, France

3:40-4:00 A Computational Model for Endocardiac Radiofrequency Ablation (RFA) with Open-Irrigated Electrodes

Luca Gerardo Giorda and Ana Gonzalez Suarez, Basque Center for Applied Mathematics, Spain; Jose M Guerra Ramos, Hospital de la Santa Creu i Sant Pau Barcelona, Spain

continued in next column

Monday, February 27

MS55

Advances in Computational Methods for Multiphysics Problems - Part II of II

2:25 PM-4:05 PM

Room:304

For Part 1 see MS26

There are many applications of multiphysics problems in material science, physics and mathematical biology. Modeling and simulating those problems, such as fluid structure interaction and conjugate heat transfer, have attracted considerable attentions from many researchers in recent years. This minisymposium aims to bring researchers together to discuss the state-of-the-art methods and algorithms, and to share the numerical challenges in the various areas.

Organizer: Longfei Li

Rensselaer Polytechnic Institute, USA

Organizer: Qi Tang

Rensselaer Polytechnic Institute, USA

2:25-2:45 A Stable Algorithm for Incompressible Flows and Rigid Bodies Based on Potentials

Qi Tang, Rensselaer Polytechnic Institute, USA

2:50-3:10 A Stable and Efficient Partitioned Algorithm for Conjugate Heat Transfer

Fanlong Meng, Jeff Banks, William Henshaw, and Donald W. Schwendeman, Rensselaer Polytechnic Institute, USA

3:15-3:35 A Numerical Study for the Arterial Intimal Thickening Based on the Reference Map Technique

Yue Yu, Lehigh University, USA; Thomas Fai, Harvard University, USA; Pak-Wing Fok, University of Delaware, USA; Chris H. Rycroft, Harvard University, USA

3:40-4:00 Multi-Implicit Discontinuous Galerkin Method for Low Mach Number Combustion

Will Pazner, Brown University, USA; Per-Olof Persson, University of California, Berkeley, USA

Monday, February 27

MS56

Recent Advances of Modeling and Computational Techniques in Biological Engineering - Part II of II

2:25 PM-4:05 PM

Room:305

For Part 1 see MS27

Mathematical modeling and computations are powerful tools for understanding the complex biological systems in bioengineering. Development of novel mathematical representations and robust computational techniques are critical for analyzing these systems. Recently, several successful attempts have been made for simulating complex biological processes like metabolic pathways, gene regulatory networks, cell signaling pathways, ion channels, cell dynamics, tumor growth, tissue engineering and biofabrication, etc. These computational-extensive models have not only reproduced experimentally verifiable phenomena, but also provided valuable insights for discovering mechanisms of the complex biological systems. This minisymposium will showcase recent progresses in developing efficient modeling and computational approaches for understanding various biological systems and their potential applications in bioengineering.

Organizer: Yi Sun

University of South Carolina, USA

Organizer: Shixin Xu

University of California, Riverside, USA

Organizer: Jia Zhao

University of North Carolina at Chapel Hill, USA

2:25-2:45 Krylov Integration Factor Method on Sparse Grids for High Spatial Dimension Convection-Diffusion-Reaction Equations

Dong Lu and *Yong-Tao Zhang*, University of Notre Dame, USA

2:50-3:10 Boundary Integral Methods for Computing Forces on Particles in Unsteady Stokes and Linear Viscoelastic Fluids

Xiaofan Li, Hualong Feng, Francisco Hernandez, and Shuwang Li, Illinois Institute of Technology, USA

3:15-3:35 An Efficient Adaptive Rescaling Scheme for Interface Problems

Meng Zhao and Shuwang Li, Illinois Institute of Technology, USA; John Lowengrub, University of California, Irvine, USA

3:40-4:00 Thermodynamically Consistent Sharp Interface Model and Fictitious Domain Method for Interaction between Fluid and Interface with Mass

Zhiliang Xu, University of Notre Dame, USA

continued in next column

Monday, February 27

MS57

Parallel Frameworks and Libraries for Tree-Structured Grids - Part II of II

2:25 PM-3:40 PM

Room:221

For Part 1 see MS28

Tree-structured computational grids have become more and more popular for various types of scientific simulations due to their advantages both in terms of fully-flexible local adaptivity and their tree-structure. The big challenges in using such grids in existing applications are 1) the effort to integrate the new grid type in a minimally-invasive while ensuring that the application inherits the advantages of the grid type in terms of memory requirements and 2) the realization of complex (and moving) geometries in the inherently Cartesian grid structure. The minisymposium presents and discusses solutions provided in frameworks and libraries addressing these two challenges.

Organizer: Miriam Mehl

Universität Stuttgart, Germany

Organizer: Carsten Burstedde

Universität Bonn, Germany

2:25-2:45 Minimally-Invasive Integration of P4est in Espresso for Adaptive Lattice-Boltzmann

Michael Lahnert and Miriam Mehl, Universität Stuttgart, Germany; Carsten Burstedde, Universität Bonn, Germany

2:50-3:10 Daino: A High-level Framework for Parallel and Efficient AMR on GPUs

Mohamed Wahib and Naoya Maruyama, RIKEN, Japan; Takayuki Aoki, Tokyo Institute of Technology, Japan

3:15-3:35 CFD Applications Using Adaptive Mesh and Space-Filling Curves on a GPU Supercomputer

Takayuki Aoki, Tokyo Institute of Technology, Japan

Monday, February 27

MS58

Measure Transport Approaches for Statistical Problems-Part II of II

2:25 PM-4:05 PM

Room:222

For Part 1 see MS29

Statistical problems such as parameter inference, data assimilation, and density estimation are ubiquitous in science and engineering. Solving these problems efficiently, however, becomes challenging with complicated datasets or nonlinear models. Recent years have seen considerable interest in tackling these problems via techniques based on nonlinear measure transformations. These transformations can be defined explicitly (e.g., via optimal transportation, Gaussianization) or implicitly via optimization (e.g., implicit filtering, randomize-then-optimize) or via the flows of ODEs. This minisymposium aims to explore connections among these measure transformation techniques and to provide a comprehensive view of their use in statistical inference and machine learning.

Organizer: Matthew Parno

US Army Cold Regions Research and Engineering Lab (CRREL), USA

Organizer: Alessio Spantini

Massachusetts Institute of Technology, USA

Organizer: Youssef M. Marzouk

Massachusetts Institute of Technology, USA

Organizer: Daniele Bigoni

Massachusetts Institute of Technology, USA

2:25-2:45 Transport Maps for Efficient Conditional Sampling

Matthew Parno, US Army Cold Regions Research and Engineering Lab (CRREL), USA; Youssef M. Marzouk, Massachusetts Institute of Technology, USA

2:50-3:10 Explanation of Variability Through Optimal Transport

Esteban G. Tabak, Courant Institute of Mathematical Sciences, New York University, USA

3:15-3:35 Dimensionality Reduction in the Wasserstein Space

Vivien Seguy, Kyoto University, Japan

3:40-4:00 Warp-Bridge Sampling to Improve Efficiency of Free Energy Calculations in Physical Chemistry

Michael Shirts, University of Colorado Boulder, USA

continued in next column

Monday, February 27

CP3

Numerical Linear Algebra - Part II of III

2:25 PM-4:05 PM

Room:223

For Part 1 see CP1
For Part 3 see CP5

Chair: Michael A. Hansen, University of Utah, USA and Sandia National Laboratories, USA

2:25-2:35 Multigrid Preconditioning for Space-Time Distributed Optimal Control of Parabolic Equations

Mona Hajghassem and Andrei Draganescu, University of Maryland, Baltimore County, USA

2:37-2:47 Spectral Matrix Analysis of the Semi-Discrete Compressible Navier-Stokes Equations Using Large-Scale Eigensolvers

Michael A. Hansen, University of Utah, USA and Sandia National Laboratories, USA; Travis Fisher, Sandia National Laboratories, USA

2:49-2:59 Why Are So Many Matrices in Computational Science of Low Rank?

Alex Townsend, Cornell University, USA; Gil Strang, Massachusetts Institute of Technology, USA

3:01-3:11 Estimating Matrix Bilinear and Quadratic Forms Using Krylov Subspace Methods with Recycling

Katarzyna Swirydowicz, Eric De Sturler, William Tyson, and Christopher Roy, Virginia Tech, USA; Misha E. Kilmer, Tufts University, USA; Xiaojia Zhang and Glaucio Paulino, Georgia Institute of Technology, USA

3:13-3:23 Multigrid Preconditioned Lattice Boltzmann Method Based on Central Moments for Efficient Computation of Fluid Flows

Farzaneh Hajabdollahi and Kannan Premnath, University of Colorado, Denver, USA

3:25-3:35 Comparison of Techniques for Hermitian Interior Eigenvalue Problems: Refined, Harmonic and Polynomial Filters

Eloy Romero Alcalde and Andreas Stathopoulos, College of William & Mary, USA

continued in next column

3:37-3:47 Fast Algorithms for Jacobi Matrices from Modification by Rational Functions

Amber C. Sumner and James V. Lambers, University of Southern Mississippi, USA

3:49-3:59 Block Triangular Preconditioners for Linearization Schemes of the Rayleigh-B\'enard Convection Problem

Guoyi Ke, Eugenio Aulisa, Giorgio Bornia, and Victoria Howle, Texas Tech University, USA

Monday, February 27

CP4

Computational Fluid Dynamics - Part II of III

2:25 PM-4:05 PM

Room:224

For Part 1 see CP2
For Part 3 see CP6

Chair: To Be Determined

2:25-2:35 Dynamic Mesh Adaptation for Front Evolution Using Discontinuous Galerkin Based Weighted Condition Number Relaxation

Patrick Greene, Samuel Schofield, and Robert Nourgaliev, Lawrence Livermore National Laboratory, USA

2:37-2:47 Computing the Ankle-Brachial Index with Computational Fluid Dynamics

John Gounley, Duke University, USA; Erik W. Draeger, Lawrence Livermore National Laboratory, USA; Jane Leopold, Brigham & Women's Hospital, USA; Amanda Randles, Duke University, USA

2:49-2:59 A DPG Method for Viscoelastic Fluids

Brendan Keith, University of Texas at Austin, USA; Philipp Knechtges, RWTH Aachen University, Germany; Nathan Roberts, Argonne National Laboratory, USA; Stefanie Elgeti and Marek Behr, RWTH Aachen University, Germany; Leszek Demkowicz, University of Texas at Austin, USA

3:01-3:11 Large Time Step HLL and HLLC Schemes

Marin Prebeg and Bernhard Müller, Norwegian University of Science and Technology, Norway

Coffee Break

4:05 PM-4:35 PM

Room:Foyer - 2nd Fl

Monday, February 27

MS59

Career Fair: Careers in Business, Industry and Government - Part III of III

4:35 PM-6:15 PM

Room:Galleria

For Part 2 see MS30

The career fair will feature employers from business, industry and government. These representatives will be prepared to discuss with you the opportunities for internships, postdoctoral appointments and full-time jobs at their organizations.

Organizer: William G. Kolata
SIAM, USA

Organizer: Kristin O'Neill
SIAM, USA

The Most Current List of Participating Companies Is Available at
http://www.siam.org/meetings/cse17/career.php

Monday, February 27

MS60

Inverse Problems Meet Big Data - Part III of III

4:35 PM-6:15 PM

Room:Grand Ballroom - 2nd Fl

For Part 2 see MS31

Inverse and big-data problems are pervasive in engineering and science. Though in past decades tremendous advances in both theories and computational algorithms for inverse problems have been made, addressing big-data issue is less common. Larger datasets implies more memory/time in processing/storing/loading. Since the amount of data we wish to process is only going to increase for the foreseeable future, there is a critical need for inverse algorithms, such as data fitting methods, that are computation- and data-scalable. This minisymposium aims to engage researchers from inverse problems and big data problems in discussions about central questions of big data inverse problems.

Organizer: Matthias Chung
Virginia Tech, USA

Organizer: Farbod Roosta-Khorasani
University of California, Berkeley, USA

Organizer: Tan Bui
University of Texas at Austin, USA

4:35-4:55 Computational Approaches for Multi-Frame Blind Deconvolution
James G. Nagy, Emory University, USA

5:00-5:20 High Performance Solvers for Linear Systems in Graph Laplacians
Richard Peng, Georgia Institute of Technology, USA; Kevin Deweese and John R. Gilbert, University of California, Santa Barbara, USA; Gary Miller, Carnegie Mellon University, USA; Serban Stan, Yale University, USA; Haoran Xu, Massachusetts Institute of Technology, USA; ShenChen Xu, Carnegie Mellon University, USA

continued in next column

5:25-5:45 Efficient MCMC Samplers for Bayesian Inverse Problems with Many Measurements
Arvind Saibaba, North Carolina State University, USA; Misha E. Kilmer, Tufts University, USA; Eric De Sturler, Virginia Tech, USA; Eric L. Miller, Tufts University, USA

5:50-6:10 Inversion Strategies for Large Scale Data and Large Scale Models
Eldad Haber, University of British Columbia, Canada

Monday, February 27

MS61

Recent Advances in Local, Adaptive, and Multilevel Uncertainty Quantification Methods for Large-Scale Scientific Computing - Part III of III

4:35 PM-6:15 PM

Room:Ballroom D - 2nd Fl

For Part 2 see MS32

Uncertainty quantification methods have seen tremendous use throughout the computational science community for enabling rigorous predictive simulation. In this minisymposium, recent advances in uncertainty quantification methods will be presented, focusing on local and adaptive methods applicable to problems involving localized behavior or discontinuities; multilevel methods exploiting hierarchies of fidelities for improved performance; and methods adapted for large-scale problems implemented on emerging extreme scale computer architectures.

Organizer: Eric Phipps

Sandia National Laboratories, USA

Organizer: Mohamed S. Ebeida

Sandia National Laboratories, USA

Organizer: Francesco Rizzi

Sandia National Laboratories, USA

4:35-4:55 Global Reconstruction of Solutions to Parametric PDEs Via Compressed Sensing

Nick Dexter, University of Tennessee, USA; Hoang A. Tran and Clayton G. Webster, Oak Ridge National Laboratory, USA

5:00-5:20 Highly Scalable Hierarchical Sampling Algorithms for Spatially Correlated Random Fields

Sarah Osborn and Panayot Vassilevski, Lawrence Livermore National Laboratory, USA

5:25-5:45 A Resilient Solver for 2D Uncertain Elliptic PDEs Via Fault-Tolerant MPI Server-Client-Based Implementation

Karla Morris and Francesco Rizzi, Sandia National Laboratories, USA; Paul Mycek, Duke University, USA; Olivier Le Maitre, LIMSI-CNRS, France; Omar M. Knio and Andres Contreras, Duke University, USA; Khachik Sargsyan, Cosmin Safta, and Bert J. Debusschere, Sandia National Laboratories, USA

5:50-6:10 Tackling UQ in Darma, a New Task-Based Programming Model for Extreme-Scale Computing

Francesco Rizzi, Eric Phipps, David Hollman, Jeremiah Wilke, Jonathan Lifflander, Hemanth Kolla, Nicole Slattengren, Keita Teranishi, and Janine C. Bennett, Sandia National Laboratories, USA

continued in next column

Monday, February 27

MS62

Advanced Modeling and Algorithms in Multiscale Problems

4:35 PM-5:50 PM

Room:202

Multiscale problems are challenging algorithmically and taxing computationally. Since the interface or boundary is constantly changing nonlinearly, accurate representation in a stable manner is not trivial, not to mention nonlinearities in the governing equations. Hence, high order and high-fidelity discretization methods combined with accurate and stable coupling strategies are needed, and analysis tools as well as acceleration (stabilization) techniques are of critical importance. In this minisymposium, we will review a number of new ideas for developing efficient and reliable multiscale methods and share interesting applications in various engineering and science fields.

Organizer: Yue Yu

Lehigh University, USA

Organizer: Xingjie Li

University of North Carolina, Charlotte, USA

4:35-4:55 Grain Growth Modeling and Novel Data Analytics for Weld Process

John A. Mitchell, Sandia National Laboratories, USA

5:00-5:20 Concurrent Multiscale Coupling Methods for the Discretized Peridynamic Theory and the Finite Element Method

Yue Yu, Lehigh University, USA; Fabiano Bargos, University of São Paulo, Brazil; Marco Bittencourt, Universidade de Campinas, Brazil; Michael L. Parks, Sandia National Laboratories, USA; George E. Karniadakis, Brown University, USA

5:25-5:45 Immersed Boundary Peridynamics Method (IB/PD) for Modeling Aortic Dissection

Amneet P.S. Bhalla, University of North Carolina at Chapel Hill, USA

Monday, February 27

MS63

Tensor Completion Techniques in Data Assimilation, Bayesian Updata and UQ Problems

4:35 PM-6:15 PM

Room:203

During last few years a lot of research was devoted to development of very efficient multi-linear algebra algorithms for tensor completion. One can see a large overlap between 1) tensor completion, 2) data assimilation and 3) Bayesian update techniques. Typical applications we keep in mind are multi-parametric PDEs, PDEs with uncertain coefficients and inverse problems. All these problems can be high dimensional and, therefore, require efficient tensor methods with (almost) linear complexity. Bayesian update and data assimilation techniques are very vital for UQ-problems and allow us to reduce uncertainties. Since stochastic dimension is usually very high all these problems (1)-(3) become very high-dimensional and all ingredients are high-dimensional tensors. In the real-life one may have only few measurements, these measurements can be very expensive or the available measurements could be far away from the quantity of interest and the question which we asking is how to complete a very sparse measurement tensor. The goal of this minisymposia is to bring experts from tensor community, Bayesian update, UQ and data assimilation together and look how the latest tensor completion techniques could be useful in applied-research areas above.

Organizer: Alexander Litvinenko
King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: Mike Espig
RWTH Aachen University, Germany

Organizer: Ivan Oseledets
Skolkovo Institute of Science and Technology, Russia

Organizer: Hermann G. Matthies
Technische Universität Braunschweig, Germany

4:35-4:55 Tensor Completion in Bayesian Inverse Problems

Alexander Litvinenko, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Hermann Matthies, Technische Universität Braunschweig, Germany

5:00-5:20 Optimization Methods on Low-Rank Manifolds and their Efficient Implementation

Ivan Oseledets, Skolkovo Institute of Science and Technology, Russia

5:25-5:45 An Efficient Method for Statistical Learning by Means of Tensor Format Representations

Mike Espig, RWTH Aachen University, Germany

5:50-6:10 Tensor Completion with Applications to Multidimensional Inverse Problems

Wojciech Czaja, University of Maryland, College Park, USA

continued in next column

Monday, February 27

MS64

Batched Linear Algebra on Multi/Many-Core Architectures

4:35 PM-6:15 PM

Room:204

The past few decades have seen a tremendous amount of effort expended on the design and implementation of software aiming to solve increasingly large-scale problems. However, many modern methods instead solve multiple small linear algebra subproblems and collate the solutions to answer the larger problem. Examples of such applications include computational fluid dynamics, image processing, metabolic network analysis, astrophysics, and machine learning. For such problems, even the use of well optimized linear algebra kernels leads to poor performance. To tackle this issue libraries such as cuBLAS, MAGMA, and MKL have begun to offer APIs for batched linear algebra computations, optimized for small problems. However, these APIs are rather immature and differ from one another significantly: there is significant room for improvement in terms of both performance and ease of use. This minisymposium is an opportunity to discuss applications, implementations, and performance results of batched linear algebra computation on current and emerging hardware. It is also a venue to discuss the standardization of batched linear algebra APIs among different library vendors. Finally, we hope to raise the profile of batched linear algebra and its potential performance benefits within the wider computational science community.

Organizer: Mawussi Zounon
University of Manchester, United Kingdom

Organizer: Pedro Valero-Lara
University of Manchester, United Kingdom

continued on next page

4:35-4:55 Recent Advances in Batched Linear Algebra Computation
Samuel Relton, Mawussi Zounon, and Pedro Valero-Lara, University of Manchester, United Kingdom

5:00-5:20 Optimizing Batched Linear Algebra on Intel(R) Xeon Phi(TM) Processors
Sarah Knepper, Murat E. Guney, Kazushige Goto, Shane Story, Arthur Araujo Mitrano, Timothy B. Costa, and Louise Huot, Intel Corporation, USA

5:25-5:45 Extending Batched GEMM for Tensor Contractions on GPU
Cris Cecka, NVIDIA, USA

5:50-6:10 Batch Linear Algebra for GPU-Accelerated High Performance Computing Environments
Ahmad Abdelfattah, University of Tennessee, Knoxville, USA

Monday, February 27

MS65

Time Domain Decomposition for PDE-Constrained Optimization

4:35 PM-6:15 PM

Room:205

The efficient solution of optimization problems constrained by time-dependent PDEs is important for many applications. The decomposition of the time domain allows to solve hard and unstable problems that can not be tackled on the entire time span. Moreover, time domain decomposition introduces another level of parallelism beyond the one used in the implementation of the underlying time-stepping. This minisymposium brings together researchers to discuss new developments and applications in this field. Important topics include new gradient-type methods, preconditioners, and model order reduction.

Organizer: Doerte Jando
Heidelberg University, Germany

Organizer: Matthias Heinkenschloss
Rice University, USA

4:35-4:55 Reduced Order Modeling for Time-Dependent Optimization Problems with Initial Value Controls
Doerte Jando, Heidelberg University, Germany; Matthias Heinkenschloss, Rice University, USA

5:00-5:20 Preconditioners for Time-Dependent PDE-Constrained Optimization Based on Parareal Time-Domain Decomposition
Stefan Ulbrich, Technische Universität Darmstadt, Germany

5:25-5:45 Parallel in Time Solutions of Variational PDE-Based Inference
Adrian Sandu, Virginia Tech, USA; Vishwas Rao, University of Texas at Austin, USA

5:50-6:10 Inexact Parallel-in-Time Solvers and SQP Methods for PDE-Constrained Optimization
Denis Ridzal, Sandia National Laboratories, USA

Monday, February 27

MS66

Smooth, Reduced, Sparse -- Exploiting Structures for Surrogate Modeling in CSE - Part III of III

4:35 PM-6:15 PM

Room:206

For Part 2 see MS37
This minisymposium explores and highlights techniques that exploit structures in computationally expensive high-fidelity models to derive accurate low-cost surrogate models. A prominent example is projection-based model reduction, which exploits that states of the high-fidelity model can be approximated well in a reduced space of low dimension. Other methods exploit the smoothness of functions that are induced by the high-fidelity model (e.g., input-output and parameter-output maps), or sparsity of representations of the high-fidelity model outputs in well-chosen bases.

Organizer: Benjamin Peherstorfer
Massachusetts Institute of Technology, USA

Organizer: Gianluigi Rozza
SISSA-ISAS International School for Advanced Studies, Italy

4:35-4:55 Improving Sparse Recovery Guarantee for Legendre Expansions Using Envelope Bound
Clayton G. Webster and *Hoang A. Tran*, Oak Ridge National Laboratory, USA

5:00-5:20 Compressed Sensing Methods for Sparse Approximations of High-Dimensional Parametric PDEs
Jean-Luc Bouchot, RWTH Aachen, Germany

5:25-5:45 Low-Rank Structure in Measure Transport for Bayesian Inference
Daniele Bigoni, Alessio Spantini, and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

5:50-6:10 Random Sketching for Projection Based Model Order Reduction
Oleg Balabanov and Anthony Nouy, Ecole Centrale de Nantes, France

Monday, February 27

MS67

Numerical Methods for Wave Propagation in Variable Media

4:35 PM-6:15 PM

Room:209

Numerical methods for solving variable coefficient partial differential equations are crucial for many applications, ranging from seismic imaging, to plasma probing, to metamaterial design. This minisymposium will gather contributions from different communities, from Dicsontinuous Galerkin to Integral Equations, to propose an overview of the variety of methods recently developed to tackle challenging problems in variable media wave propagation.

Organizer: Lise-Marie Imbert-Gerard

Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Leonardo Zepeda-Nunez

University of California, Irvine, USA

4:35-4:55 An Efficient High Accuracy Direct Solution Technique for High Frequency Helmholtz Problems

Adrianna Gillman, Rice University, USA

5:00-5:20 A Fast and High-Order Hybridizable Discontinuous Galerkin Solver for the High-frequency Helmholtz Equation

Matthias Taus, Massachusetts Institute of Technology, USA; Leonardo Zepeda-Nunez, University of California, Irvine, USA; Laurent Demanet, Massachusetts Institute of Technology, USA

5:25-5:45 Learning Dominant Wave Directions For Plane Wave Methods For High-Frequency Helmholtz Equations

Jun Fang, University of California, Irvine, USA

5:50-6:10 A Simple Curved Boundary Treatment for Explicit High Order Dg Methods Solving Time-Dependent Problems

Xiangxiong Zhang, Purdue University, USA

Monday, February 27

MS68

Uncertainty Quantification for Computational Fluid Dynamics in Sustainable Energy Applications

4:35 PM-6:15 PM

Room:210

For more than a decade already, uncertainty quantification (UQ) is of growing relevance for various computational fluid dynamics (CFD) problems, particularly in the area of sustainable energy. An example of an important UQ application area in this respect is offshore wind-farm (OWF) aerodynamics. A proper design, construction and operation of OWFs must deal with uncertainties in, e.g., weather conditions, and their effects on turbine blade loading and power production, when numerically simulating the aerodynamics of wind turbine wakes and the structural dynamics of the blades. Main challenges in this are: (i) to determine and parameterize the various uncertainties that play a role in OWF aerodynamics, (ii) to calibrate the mathematical-physical models (such as turbulence models) based on measurement data or high-fidelity models, and (iii) to determine how uncertainties propagate through the models and influence the quantity of interest, such as the cost of energy. In this minisymposium we bring together researchers to discuss and learn about dealing with this type of problems: calibration and propagation of uncertainties in high dimensional random parameter spaces, combined with high computational cost associated with model runs directed towards sustainable energy applications.

Organizer: Barry Koren

Eindhoven University of Technology, Netherlands

4:35-4:55 Bayesian Calibration of Model-Form Uncertainty Applied to Wind Turbine Wake Simulation

Laurent van den Bos and Benjamin Sanderse, Centrum voor Wiskunde en Informatica (CWI), Netherlands

5:00-5:20 A Method for Data-Assimilation in Navier-Stokes with a Least-Squares Rom

Richard P. Dwight, Delft University of Technology, Netherlands

5:25-5:45 UQ for Correlated Inputs

Anne Eggels, Centrum voor Wiskunde en Informatica (CWI), Netherlands; Daan Crommelin, University of Amsterdam, Netherlands

5:50-6:10 UQ for Particle-Laden Turbulent Flows in Solar Receivers

Lluis Jofre, Gianluca Geraci, and Gianluca Iaccarino, Stanford University, USA

continued in next column

Monday, February 27

MS70

Multifidelity Simulation and Approximation in the Computational Sciences - Part II of II

4:35 PM-6:15 PM

Room:212

For Part 1 see MS41

A modern computational mainstay is the multifidelity challenge: make efficient and robust predictions given several competing models each having its own degree of trust. The abstract concept of "fidelity" -- faithfulness to physics, experimental observations, and/or idealized mathematical formulations -- arises because different simulation suites utilize different discretization types and scales, and make dissimilar simplifications of underlying physics. This minisymposium aims to highlight recent advances in algorithms that make optimal use of models with differing fidelities. The challenges include resource distribution among models, identification and learning of model hierarchy, and efficient synthesis of model predictions.

Organizer: Akil Narayan

University of Utah, USA

Organizer: Xueyu Zhu

University of Iowa, USA

4:35-4:55 Multilevel-Multifidelity Approaches for Uncertainty Quantification and Design

Michael S. Eldred, Sandia National Laboratories, USA; Jason Monschke, Texas A&M University, USA; John D. Jakeman, Sandia National Laboratories, USA; Gianluca Geraci, Stanford University, USA

5:00-5:20 Computing Failure Probability Using Models of Different Fidelities

Yuhang Chen, Ohio State University, USA; Jing Li, Pacific Northwest National Laboratory, USA; Dongbin Xiu, Ohio State University, USA

continued in next column

5:25-5:45 Numerical Strategy for Model Correction Using Physical Constraints

YanYan He, University of Utah, USA; Dongbin Xiu, Ohio State University, USA

5:50-6:10 Stochastic Reduced Model for Multiple Scales in Porous Media

Malgorzata Peszynska, Oregon State University, USA; Timothy B. Costa, Intel Corporation, USA

Monday, February 27

MS71

Recent Advance on Numerical Methods for Quantum Problems - Part III of III

4:35 PM-6:15 PM

Room:213

For Part 2 see MS42

Quantum problems have numerous applications in quantum physics and chemistry, plasma and particle physics, material sciences, semiconductor theory, rarefied gas theory, Bose-Einstein condensation, nonlinear optics, erc. The typical models include nonlinear Schroedinger equation (NLS), Dirac equation, Klein-Gordon equation, density fucntional theory, quantum Boltzmann equation, etc. The purpose of this minisymposium is to provide a platform for the researchers in the field to present recent work on the numerical analysis, numerical methods and simulation for these quantum problems, to exchange idea and to discuss future directions in the field.

Organizer: Qinglin Tang

Université de Lorraine, France

4:35-4:55 Solid-State Dewetting: Equilibrium & Dynamics

Wei Jiang, Wuhan University, China

5:00-5:20 Multiscale Methods for Highly Oscillatory Quantum and Kinetic Problems

Xiaofei Zhao, Mohammed Lemou, and Florian Mehats, Université de Rennes 1, France; Nicolas Crouseilles, Inria Rennes, France

5:25-5:45 Numerical Methods for Solving the Fractional Schroedinger Equation

Siwei Duo, Missouri University of Science and Technology, USA

5:50-6:10 The Earthquake Location Methods Based on Waveform Inversion

Jing Chen and Hao Wu, Tsinghua University, China; Xueyuan Huang, Beijing Technology And Business University, China; Dinghui Yang, Tsinghua University, China

Monday, February 27

MS72

Time Stepping Methods for Initial Boundary Value Problems

4:35 PM-6:15 PM

Room:214

This minisymposium focuses on challenges in efficient high order time stepping particular to problems that also have spatial dimensions and/or other complex structure. Particular focal points include: order-reduction for partial differential equations, unconditionally stable ImEx schemes, time-stepping for incompressible flows, and convex-concave splittings. In all of these cases, particular challenges and requirements on the time-stepping schemes arise that go beyond what one is used to from the realm of ordinary differential equations.

Organizer: David Shirokoff

New Jersey Institute of Technology, USA

Organizer: Rodolfo R. Rosales

Massachusetts Institute of Technology, USA

4:35-4:55 Unconditional Stability for Multistep Imex Schemes

David Shirokoff, New Jersey Institute of Technology, USA

5:00-5:20 Diagonally Implicit Runge-Kutta Schemes Devoid of Order Reduction

Benjamin Seibold, Temple University, USA; Rodolfo R. Rosales, Massachusetts Institute of Technology, USA; David Shirokoff, New Jersey Institute of Technology, USA; Dong Zhou, Temple University, USA

5:25-5:45 Order Reduction in Implicit Runge-Kutta Time-Stepping for Initial Boundary Value Problems

Dong Zhou, Temple University, USA; Rodolfo R. Rosales, Massachusetts Institute of Technology, USA; Benjamin Seibold, Temple University, USA; David Shirokoff, New Jersey Institute of Technology, USA

5:50-6:10 Spectral Accuracy in Time and Space for a Semi-Implicit Approach to the Incompressible Navier-Stokes Equations in Complex Geometries

Michael Minion, Lawrence Berkeley National Laboratory and Stanford University, USA; Robert Saye, Lawrence Berkeley National Laboratory, USA

Monday, February 27

MS73

Numerical Methods for PDEs on Surfaces

4:35 PM-5:50 PM

Room:215

Partial differential equations posed on surfaces arise in mathematical models for many natural phenomena: diffusion along grain boundaries, lipid interactions in biomembranes, pattern formation, and transport of surfactants on multiphase flow interfaces to mention a few. Numerical simulations play an increasingly important role in a better understanding and prediction of processes involving these or other surface phenomena. This featured minisymposium focuses on most recent developments of numerical techniques dealing with PDEs posed on manifolds and applications of these methods in natural and applied sciences. The leaders in the field will explore the state of the art and discuss future challenges.

Organizer: Maxim A. Olshanskii

University of Houston, USA

4:35-4:55 Unfitted Finite Element Methods for PDEs on Evolving Surfaces

Maxim A. Olshanskii, University of Houston, USA

5:00-5:20 A High Order Trace Finite Element Method for PDEs on Level Set Surfaces

Arnold Reusken and Joerg Grande, RWTH Aachen University, Germany; Christoph Lehrenfeld, Universität Münster, Germany

5:25-5:45 An Embedding Method for PDEs on Moving Surfaces

Argyrios Petras and *Steven Ruuth*, Simon Fraser University, Canada

Monday, February 27

MS74

In Situ Methods and Infrastructures: Faster Insight Through Smarter Computing

4:35 PM-6:15 PM

Room:216

IO is increasingly becoming a bottleneck for HPC simulations. This is due to the widening gap between available FLOPs and IO rates. In situ processing, where analysis and visualization output is concurrently generated with the running simulation, has been shown to be a useful technique to overcome this IO bottleneck. While in situ processing has a long history in scientific computing, there are a variety of production quality tools now available. In addition, a significant amount of work is currently focused on user issues and scaling to exascale. This includes a focus on efficiently sharing HPC system resources with the simulation to ensure that in situ output does not negatively impact the simulation run.

Organizer: Andrew C. Bauer

Kitware, Inc., USA

Organizer: E. Wes Bethel

Lawrence Berkeley National Laboratory, USA

4:35-4:55 In Situ Processing Overview and Relevance to the HPC Community

E. Wes Bethel, Lawrence Berkeley National Laboratory, USA

5:00-5:20 SENSEI: A Lightweight In Situ Interface for Contemporary Infrastructure Tools and Architectures

Andrew C. Bauer, Patrick O'Leary, and Utkarsh Ayachit, Kitware, Inc., USA

5:25-5:45 Extract Based In Situ Visualization and Analysis Methods and Application to Engineering Simulations

Earl P. N. Duque, Intelligent Light, USA; *Brad Whitlock*, Lawrence Livermore National Laboratory, USA

5:50-6:10 Master of Puppets: Cooperative Multitasking for In Situ Processing

Erich Lohrmann, Georgia Institute of Technology, USA; Zarija Lukic, Dmitriy Morozov, and Juliane Mueller, Lawrence Berkeley National Laboratory, USA

Monday, February 27

MS75

Model Reduction Software: Nonlinear Problems and Data-Driven Solutions

4:35 PM-6:15 PM

Room:217

To accelerate the repeated simulation of large-scale models based on differential equations, the discipline of model reduction provides algorithms for the approximation by surrogates with lower computational complexities. For complex nonlinear models, an active field of research are data-driven model reduction techniques, that utilize simulation or measurement data to construct the reduced order models. The practical computations are performed by model reduction software, which for nonlinear models faces additional challenges such as lifting. This minisymposium discusses current research on data-driven nonlinear model order reduction methods and its software implementations.

Organizer: Christian Himpe

Max Planck Institute, Magdeburg, Germany

4:35-4:55 Regularization Techniques for Biochemical Reaction Networks

Daniel Howsmon and Juergen Hahn, Rensselaer Polytechnic Institute, USA

5:00-5:20 Nonlinear Model Order Reduction with pyMOR

Stephan Rave, Universität Münster, Germany

5:25-5:45 Data-Driven Methods for Nonlinear Model Reduction in Fluid Dynamics

Scott Dawson and Clarence Rowley, Princeton University, USA

5:50-6:10 Model Reduction Via Spectral Analysis of the Koopman Operator

Ryan Mohr, University of California, Santa Barbara, USA

Monday, February 27

MS76

Emerging Consensus in Code Generation Approaches for Finite Element Methods

4:35 PM-6:15 PM

Room:218

The increasing complexity of hardware, numerics and applications for simulation science has created rapidly increasing interest in code generation as a mechanism for combining high level, high productivity user environments with high performance low level implementations. In particular, the Unified Form Language and the surrounding FEniCS problem solving language are emerging as a de facto standard among a number of high level finite element frameworks. This minisymposium will feature contributions from the FEniCS, Firedrake, DUNE-FEM and DUNE-PDELab projects focussing on the recent developments in code generation from the Unified Form Language to the diverse implementation approaches and numerical capabilities of these platforms. The minisymposium will contribute to the ongoing multiway dialogue between the developers and users of these and other finite element platforms with the objective of converging on high level interfaces which capture the abstract mathematical structure of a maximal set of numerical approaches and application areas.

Organizer: David Ham

Imperial College, United Kingdom

4:35-4:55 The Two-Stage Form Compiler, a Mechanism for Structure-Preserving Code Generation

Miklós Homolya, Lawrence Mitchell, and Fabio Luporini, Imperial College London, United Kingdom; David Ham, Imperial College, United Kingdom

5:00-5:20 Using Code Generation to Improved Performance of a Multipurpose Discontinuous Galerkin Implementation Based on Dune-Fem

Robert Klöfkorn, International Research Institute of Stavanger (IRIS), Norway

5:25-5:45 The Unified Form Language and Key Points on its Translation

Martin Alnæs, Simula Research Laboratory, Norway

5:50-6:10 Generating Performance-Optimized Fem Assembly Kernels for Dune-Pdelab

Dominic Kempf, René Heß, Steffen Müthing, and Peter Bastian, Universität Heidelberg, Germany

continued in next column

Monday, February 27

MS77

High-Performance Hybrid Programming

4:35 PM-6:15 PM

Room:219

As high performance computing architectures become more complex, with heterogeneous processing elements and deeper memory hierarchies, multiple approaches to parallel programming are needed. The focus of this minisymposium is on hybrid programming models, including the benefits and limitations as algorithms adapt to mixed models. In particular, MPI everywhere, OpenMP+MPI, as well as CPU+Device models are considered in a range of talks that cover algorithms, performance models, and software stacks.

Organizer: Luke Olson

University of Illinois at Urbana-Champaign, USA

Organizer: William D. Gropp

University of Illinois at Urbana-Champaign, USA

4:35-4:55 Efficient MPI-Openmp Programming for Scientific Applications

William D. Gropp, Luke Olson, and Philipp Samfass, University of Illinois at Urbana-Champaign, USA

5:00-5:20 Preconditioning on Parallel and Hybrid Architectures

Hartwig Anzt, University of Tennessee, USA; Thomas K. Huckle, Technische Universität München, Germany; Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA

5:25-5:45 OCCA : Open Concurrent Compute Abstraction

Tim Warburton, Virginia Tech, USA; David Medina, Rice University, USA

5:50-6:10 Extending Kokkos for Task-Parallel and Structured Grid Algorithms with Asynchronous Parallelism

Daniel Sunderland, Sandia National Laboratories, USA

Monday, February 27

MS78

Selected Inversion and Its Application

4:35 PM-6:15 PM

Room:220

Selected inversion is a technique for computing selected elements of the inverse of a sparse matrix A without computing the entire inverse. This type of computation is the key to reducing the complexity of Kohn-Sham density functional theory based electronic structure calculations, Green's function based electron transport calculations, quantitative genetics and many other scientific applications. Although the original algorithm for performing selected inversion was proposed in the 70's, high performance implementation of this algorithm on shared and distributed memory parallel computers became available only recently. This minisymposium aims to highlight the recent algorithmic development of selected inversion and its high performance implementation, as well as applications that can make effective use of selected inversion.

Organizer: Chao Yang

Lawrence Berkeley National Laboratory, USA

Organizer: Olaf Schenk

Università della Svizzera italiana, Switzerland

4:35-4:55 Scalable Selective Inversion and Stochastic Estimation of Inverse Matrices

Fabio Verbosio, Università della Svizzera italiana, Switzerland; Matthias Bollhoefer, Technische Universität Braunschweig, Germany; Olaf Schenk, Università della Svizzera italiana, Switzerland

5:00-5:20 Recent Development of the Parallel Selected Inversion Method on Many-Core Architecture

Weile Jia, University of California, Berkeley, USA

5:25-5:45 Selected Inversion in Quantitative Genetics

Yataka Masuda, University of Georgia, USA

5:50-6:10 A Hybrid Method for Computing Selected Entries of Matrix Inverse

Song Li, Stanford University, USA

Monday, February 27

MS79

Numerical Reproducibility

4:35 PM-6:15 PM

Room:Crystal AF - 1st Fl

A cornerstone of the scientific method is experimental reproducibility. As computation has grown into a powerful tool for scientific inquiry, the assumption of computational reproducibility has been at the heart of numerical analysis in support of scientific computing. With ordinary CPUs, supporting a single, serial, computation, the ability to document a numerical result has been a straightforward process. However, as computer hardware continues to develop, it is becoming harder to ensure computational reproducibility, or to even completely document a given computation. This minisymposium will explore the current state of computational reproducibility in computational science. In addition, this minisymposium is a companion to the Numerical Reproducibility at Exascale workshop held annually at the SCXX meetings.

Organizer: Michael Mascagni

Florida State University, USA

4:35-4:55 An Overview of Lessons Learned at the Numerical Reproducibility at Exascale Workshops

Walid Keyrouz, National Institute of Standards and Technology, USA

5:00-5:20 The Forensic Reproducibility of Pseudorandom Number Generation on Modern Architectures

Michael Mascagni, Florida State University, USA

5:25-5:45 Reproducibility of Stochastic Methods for Computing Material Properties

Derek Juba, National Institute of Standards and Technology, USA

5:50-6:10 The Numerical Reproducibility Fair Trade: Facing the Concurrency Challenges at the Extreme Scale

Michela Taufer, University of Delaware, USA

Monday, February 27

MS80

Model Discrepancy and Model Form Error Approaches: Intrusive Approaches

4:35 PM-6:15 PM

Room:Crystal CD - 1st Fl

Model discrepancy is defined as the difference between model predictions and experimental data, sometimes called "model form error" or "structural model error". There are a variety of approaches being developed, including formulations that represent discrepancy explicitly using, for example, Gaussian processes or polynomial chaos expansions, as well as implicit formulations in which "model correction" terms are determined concurrently with the solution of a set of partial differential equations. Approaches that are Bayesian or non-Bayesian in nature, along with those supported by machine learning principles, may be used to estimate model discrepancy. This minisymposium focuses mainly on intrusive formulations and is meant to foster discussion of the various methods.

Organizer: Yan Wang

Georgia Institute of Technology, USA

4:35-4:55 Determination of Model Form Uncertainties Using Field Inference and Machine Learning

Karthik Duraisamy, University of Michigan, Ann Arbor, USA

5:00-5:20 Reducing Model Discrepancy in Turbulent Flow Simulations: A Physics-Informed Machine Learning Approach

Jinlong Wu, Jianxun Wang, and Heng Xiao, Virginia Tech, USA

5:25-5:45 A Stochastic Operator Approach to Model Inadequacy with Applications to Contaminant Transport

Teresa Portone, Damon McDougall, Robert D. Moser, and Todd A. Oliver, University of Texas at Austin, USA

5:50-6:10 Parameter Identification of a Counter Flow Heat Exchanger with Physics Based Model-Form Discrepancy

John A. Burns and Eugene Cliff, Virginia Tech, USA

Monday, February 27

MS81

Statistical Models and Monte Carlo Schemes for Inverse Problems in Imaging

4:35 PM-5:50 PM

Room:301

Inverse problems are typically characterized by estimating a large number of unknowns from indirectly related data corrupted by stochastic effects such as measurement. Usually, inverting the process modeling the data is unstable with respect to these effects and requires incorporation of a priori knowledge or regularization to stabilize the estimation. In imaging science in particular, the data is often large scale and the models exhibit problematic instability. Moreover, in order for estimates to be meaningful, they must also include quantification of the uncertainty involved in obtaining them. State of the art techniques from statistics and stochastic modeling provide methods to overcome both of these difficulties, and this minisymposium will focus on their specific application to problems in imaging science for estimation and quantification of uncertainty.

Organizer: Kevin Joyce

Nevada National Security Site, USA

Organizer: Aaron B. Luttman

National Security Technologies, LLC, USA

4:35-4:55 Point Spread Function Estimation Using Radially Symmetric Prior Modeling and Enhanced Gibbs Sampling

Kevin Joyce, Nevada National Security Site, USA; Johnathan M. Bardsley, University of Montana, USA; Aaron B. Luttman, National Security Technologies, LLC, USA

5:00-5:20 Wavelet Estimators of Multivariable Nonparametric Regression Functions with Long Memory Data

Dongsheng Wu and Yunzhu He, University of Alabama, Huntsville, USA

5:25-5:45 Multilevel Monte Carlo Algorithms for Inference

Kody Law, Oak Ridge National Laboratory, USA

Monday, February 27

MS82

Integral Equation Methods for Inhomogeneous Partial Differential Equations

4:35 PM-6:15 PM

Room:302

Integral equation methods have been shown to be both highly accurate and efficient when solving homogeneous constant coefficient elliptic partial differential equations in complex geometry. Much current research is focused on extending their applicability to problems with variable coefficients, inhomogeneous source terms, time dependence and nonlinearities. This will require the creation of new tools to address issues including quadrature design, function extension and the rapid evaluation of volume potentials. This minisymposium will highlight some of these developments.

Organizer: Leslie Greengard

Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Anna-Karin Tornberg

KTH Royal Institute of Technology, Sweden

4:35-4:55 Smooth Function Extension for the Solution of Inhomogeneous Equations in Complex Geometry

Anna-Karin Tornberg, KTH Royal Institute of Technology, Sweden

5:00-5:20 Fast Methods for the Evaluation of Heat Potentials in Moving Geometry

Jun Wang, New York University, USA

5:25-5:45 Integral Equation Methods for Nonlinear Fluid Models

Shravan Veerapaneni, University of Michigan, USA

5:50-6:10 An Adaptive Fast Multipole Accelerated Poisson Solver for Complex Geometries

Antoine Cerfon, New York University, USA; Travis Askham, University of Washington, USA

Monday, February 27

MS83

Small-Scale Flows with Industrial Applications: Modeling and Simulations

4:35 PM-6:15 PM

Room:303

Challenging mathematical problems involving fluid dynamics at small scales, often with attendant particle transport, can be found in many real-world scientific, engineering and industrial applications. Such problems are usually very complicated to solve due to the complexity of the governing equations and the need to deal accurately with the particles; and the complexity can increase further as the system size shrinks, therefore flow and particle transport on the micro or nano scale has to be considered. Mathematical modeling and asymptotic analysis can play a key role in simplifying many industrial problems, particularly in cases where the full governing equations require computational fluid mechanics and molecular dynamics simulations, which are extremely computationally expensive. In this minisymposium we introduce several closely-related applied mathematical problems in fluid mechanics, relating to membrane filtration, micro-fluidic devices and diffusion of nano particles. We consider a variety of approaches to these problems, ranging from asymptotic approaches to derive simplified models that are relatively cheap to solve, through to sophisticated computational physics simulations.

Organizer: Pejman Sanaei
New Jersey Institute of Technology, USA

4:35-4:55 Mathematical Modeling of Pleated Membrane Filters
Pejman Sanaei, New Jersey Institute of Technology, USA; Giles Richardson, University of Southampton, United Kingdom; Thomas P. Witelski, Duke University, USA; Linda Cummings, New Jersey Institute of Technology, USA

5:00-5:20 Modeling Flow Rate--Pressure Drop Relations of Soft Micro-Fluidic Devices
Ivan C. Christov and Tanmay Shidhore, Purdue University, USA

5:25-5:45 Molecular Dynamics Simulation Study of the Diffusion of a Janus Nano-Particle in an Explicit Solvent
Ali Kharazmi, Michigan State University, USA; Nikolai Priezjev, Wright State University, USA

5:50-6:10 Growth of Clogs in Microchannels: Formation of the Filter Cake
Emilie Dressaire, New York University, USA

continued in next column

Monday, February 27

MS84

Domain-Specific Abstractions for Full-Waveform Inversion

4:35 PM-6:15 PM

Room:221

Full-waveform inversion is a PDE-constrained optimisation problem involving massive amounts of data (petabytes) and large numbers of unknowns ($O(10^9)$). This well known compute-intensive and data-intensive is extremely challenging for several reasons. First, there is the complexity of having to handle extremely large data volumes with metadata related to experimental details in the field, and the discretization of the unknown earth parameters and approximate physics. Second, reduced or adjoint-state methods call for computationally intensive PDE solves for each source experiment (of which there are thousands) for each iteration of a gradient-based optimization scheme. The talks will give an overview how carefully chosen layers of abstraction can help manage both the complexity and scale of inversion while still achieving the high degree of computational performance required to make full-waveform a practical tool. Specifically, the presentations will focus on domain specific stencil language for time-stepping methods to solve various types of wave equations and on abstracts for large-scale parallel optimization frameworks.

Organizer: Felix J. Herrmann
University of British Columbia, Canada

Organizer: Gerard J. Gorman
Imperial College London, United Kingdom

4:35-4:55 Considerations and Techniques for Optimizing HPC Stencil Performance on the Intel® Xeon Phi™ Processor
Charles Yount, Intel Corporation, USA

continued on next page

5:00-5:20 Symbolic Math for Automated Fast Finite Difference Computations

Navjot Kukreja, SENAI CIMATEC, Brazil

5:25-5:45 Multi-Physics Geophysical Exploration: Raising the Abstraction with Separation of Concerns

Mathias Louboutin, University of British Columbia, Canada

5:50-6:10 Large-Scale Workflows for Wave-Equation Based Inversion in Julia

Philipp A. Witte, University of British Columbia, Canada

Monday, February 27

MS289

Programming Models and Libraries for Modernizing Legacy Applications for Exascale

4:35 PM-6:15 PM

Room:211

Data explosion termed as big data is applicable in all scientific fields, climate change, cancer illness, national nuclear security. We need powerful machines to calculate, analyze, compute and process abundance amounts of data, which will only continue to grow. At the same time, we also need to modernize legacy code such that they can exploit different levels of parallelism offered by these massively parallel machines. To that end, this symposium discusses different ways to modernize legacy code on extreme scale systems specifically using OpenMP, OpenACC, Kokkos, Legion and other libraries. The talks will focus on strategies for programming abstraction, interoperability, performance portability, memory management and extensibility. Some models allow applications to identify parallelizable grains of computations and data and let the library map them to cores and data to memory; other models are still evolving to provide vocabulary for data layout and memory space. Choosing different data layout without modifying users' computational code can be a real challenge and a pressing concern given varied hardware types. The talks will assess the effectiveness and impact of design decisions using critical scientific miniapps. This session will highlight convergence between life sciences and computer science investigating how the current parallel computing technologies can address the vast computing challenges in legacy code on extreme scale systems.

Organizer: Sunita Chandrasekaran

University of Delaware, USA

continued in next column

Organizer: Jakub Kurzak

University of Tennessee, USA

Organizer: Patrick McCormick

Los Alamos National Laboratory, USA

Organizer: Christian Trott

Sandia National Laboratories, USA

4:35-4:55 Exploring On-Node Programming Models for Irregular Algorithms

Sunita Chandrasekaran, University of Delaware, USA

5:00-5:20 Interoperability, Portability and Productivity Challenges for Transforming Legacy Applications

Patrick McCormick, Los Alamos National Laboratory, USA

5:25-5:45 Preparing Sandia's Application Portfolio for the Future Using Kokkos

Christian Trott, Daniel Sunderland, Simon D. Hammond, and H. Carter Edwards, Sandia National Laboratories, USA

5:50-6:10 Dense Linear Algebra at Exascale: Challenges and Opportunities

Jakub Kurzak, University of Tennessee, USA

Monday, February 27

CP5

Numerical Linear Algebra - Part III of III

4:35 PM-6:15 PM

Room:223

For Part 2 see CP3

Chair: Haley Dozier, University of Southern Mississippi, USA

4:35-4:45 Multigrid Preconditioning of Linear Systems Arising in the Semismooth Newton Solution of Distributed Optimal Control of Elliptic Equations with State Constraints

Jyoti Saraswat, Thomas More College, USA; Andrei Draganescu, University of Maryland, Baltimore County, USA

4:47-4:57 Multigrid Kss Methods for Time-Dependent PDEs

Haley Dozier and James V. Lambers, University of Southern Mississippi, USA

4:59-5:09 Inexact Algebraic Factorization Methods for the Steady Incompressible Navier-Stokes Equations

Alex Viguerie and Alessandro Veneziani, Emory University, USA

5:11-5:21 Investigations of Several Mhd Solvers Based on Discontinuous Galerkin Finite Element Method

Xiaohe Zhufu, Chinese Academy of Sciences, China; Yanfei Jiang, Harvard University, USA; Zhaoming Gan, Defu Bu, Maochun Wu, and Jin Xu, Chinese Academy of Sciences, China

5:23-5:33 Automatic Construction of Scalable Time-Stepping Methods for Stiff Pdes

Vivian A. Montiforte and James V. Lambers, University of Southern Mississippi, USA

Monday, February 27

CP6

Computational Fluid Dynamics - Part III of III

4:35 PM-6:15 PM

Room:224

For Part 2 see CP4

Chair: To Be Determined

4:35-4:45 Energy Conservation Moment Method to Solve the Multi-Dimensional Vlasov-Maxwell-Fokker-Planck Equations

Yanli Wang, Institute of Applied Physics and Computational Mathematics, China

4:47-4:57 DOF-Reducing Small-Lebesgue Polygonal Spectral Basis Functions with Application to Discontinuous FEM

Arash Ghasemi, University of Tennessee, Chattanooga, SimCenter, USA

4:59-5:09 A Hybrid Adaptive Compressible/Low-Mach-Number Method

Emmanuel Motheau, Ann S. Almgren, and John B. Bell, Lawrence Berkeley National Laboratory, USA

5:11-5:21 An Arbitrary High Order Imex Scheme For Extended Magnetohydrodynamics Equations Using Entropy Conservative Flux

Chhanda Sen and Harish Kumar, Indian Institute of Technology, Delhi, India

SINUM Dinner Meeting (by invitation only)

7:00 PM-10:00 PM

Room:Crystal BE - 1st Fl

Tuesday, February 28

Registration

7:00 AM-5:00 PM

Room:Foyer - 1st Fl

Announcements

8:10 AM-8:15 AM

Room:Grand Ballroom - 2nd Fl

Tuesday, February 28

IP3

Ingredients for Computationally Efficient Solution of Large-Scale Image Reconstruction Problems

8:15 AM-9:00 AM

Room:Grand Ballroom - 2nd Fl

Chair: Michele Benzi, Emory University, USA

Image reconstruction problems provide great opportunities to bring together many scientific computing techniques to advance the state of the art in inverse problems and in disciplinary areas. First, we need to tailor the inverse problem to the application to produce the regularized solution while considering how a priori knowledge is enforced. We might choose to enforce hard constraints, like non-negativity, sparsity and/or high-contrast. Alternatively, we may choose to employ a learned dictionary or a parameterized image model that imposes those constraints directly on image space and simultaneously restrict the search space. Second, those modeling choices, which are interesting problems in and of themselves, necessitate the use of sophisticated optimization algorithms. Third, since each optimization step requires multiple forward model simulations, techniques from the multigrid, model reduction and randomization communities need to be explored to attain the maximum computational efficiency. In this talk, we provide an overview of some of these scientific computing techniques that have been successfully used in image reconstruction, and provide some combinations of techniques that have led to particularly fruitful outcomes in the context of a few applications.

Misha E. Kilmer
Tufts University, USA

Intermission

9:00 AM-9:10 AM

Tuesday, February 28

MT3

CSE Collaboration through Software: Improving Productivity and Sustainability- Part I

9:10 AM-10:50 AM

Room:Ballroom C - 2nd Fl

For Part 2 see MT4

Chair: Lois Curfman McInnes, Argonne National Laboratory, USA

CSE software—crosscutting technology that connects advances in mathematics, computer science, and domain-specific science and engineering—is a foundation of sustained CSE collaboration and scientific progress. However, the need for increasingly broad functionality on ever more complex computer architectures creates daunting challenges for software development and sustainability. This tutorial will provide information on best practices in software engineering explicitly tailored for CSE. Goals are improving the productivity of those who develop CSE software and increasing the sustainability of software artifacts. We will discuss practices that are relevant for projects of all sizes, with emphasis on small teams (for example, a faculty member and collaborating students). Part 1: Why effective software practices are essential for CSE projects; understanding what you want from your CSE software and how to achieve it; software testing; integrated software lifecycle. Part 2: Software licensing; effective models, tools, processes, and practices for small software teams; how to collaborate (around code) with people outside your domain; agile workflow management for small teams. Target attendees include CSE investigators who develop software and people who plan and fund CSE projects that incorporate software. The tutorial will incorporate interactive exercises, including a walk through of small team and agile activities for an example GitHub project.

continued in next column

Speakers:

Lois Curfman McInnes
Argonne National Laboratory, USA

David E. Bernholdt
Oak Ridge National Laboratory, USA

Anshu Dubey
Argonne National Laboratory, USA

Michael Heroux
Sandia National Laboratories, USA

Alicia Klinvex
Sandia National Laboratories, USA

Tuesday, February 28

MS85

Coupling Methods in Multiphysics and Multiscale Problems - Part I of II

9:10 AM-10:50 AM

Room:Grand Ballroom - 2nd Fl

For Part 2 see MS113

There has been great interests in the computational methods for multiphysics and multiscale problems due to their importance in engineering and biomedical applications. In the numerical algorithms, information needs to be exchanged at the interface, which brings nonlinearities into the coupled system. Therefore, tackling the immanent complexity of interface and coupling strategies requires crossdisciplinary thinking, sophisticated modeling and advanced numerical methods. This minisymposium will focus on the advanced coupling strategies for multiphysics and multiscale problems. It aims at bringing together researchers from across the applied mathematics and engineering communities to discuss and exchange new ideas for developing efficient and reliable coupling algorithms, and to transfer knowledge between the two communities. Topics of interest include, but not limited to, stabilized methods for coupling frameworks, novel numerical methods for fluid-structure interaction, algorithmic aspects in biomechanics simulations, coupling between local and nonlocal models, and the complex dynamics of molecular biosciences.

Organizer: Yue Yu
Lehigh University, USA

Organizer: Xingjie Li
University of North Carolina, Charlotte, USA

continued in next column

9:10-9:30 DG-IMEX Asymptotic-Preserving Schemes and Their Stability
Fengyan Li, Rensselaer Polytechnic Institute, USA

9:35-9:55 Computational Vascular and Valvular Fluid-Structure Interaction
Ming-Chen Hsu, Iowa State University, USA; David Kamensky, University of California, San Diego, USA; Fei Xu, Iowa State University, USA

10:00-10:20 Large-Scale Fracture Simulations Using Atomistic-Based Boundary Element Method
Xiaojie Wu and Xiantao Li, Pennsylvania State University, USA

10:25-10:45 A New Poisson–Nernst–Planck Model with Ion–Water Interactions for Charge Transport in Ion Channels
Duan Chen, University of North Carolina, Charlotte, USA

Tuesday, February 28

MS87

Partial Differential Equation Techniques for Network Problems - Part I of II

9:10 AM-10:50 AM

Room:202

For Part 2 see MS114

Network problems are prevalent in image processing and data analysis, for example in image segmentation, data classification, and community detection. In recent years new approaches to such problems have been proposed, based on techniques from partial differential equations and variational methods. These approaches offer new possibilities for computationally feasible applications to large data sets, as well as exciting new theoretical connections between partial differential equations and applied analysis on the one hand and network science and graph theory on the other. This minisymposium will bring together scientists from the US and Europe who are working on both the computational and theoretical aspects of the field.

Organizer: Yves van Gennip
University of Nottingham, United Kingdom

Organizer: Carola Schönlieb
University of Cambridge, United Kingdom

9:10-9:30 Geometric Graph Methods for High Dimensional Data
Andrea L. Bertozzi, University of California, Los Angeles, USA

9:35-9:55 Primal-Dual Methods for P-Modulus on Graphs
Dominique P. Zosso, Montana State University, USA

10:00-10:20 Convex Variational Methods for Multi Class Data Segmentation on Graphs
Ekaterina Merkurjev, Michigan State University, USA; Egil Bae, University of Bergen, Norway

10:25-10:45 A Max-Cut Approximation Using A Graph Based MBO Scheme
Blaine Keetch, University of Nottingham, United Kingdom

Tuesday, February 28

MS88

Resilient PDE Solvers for (Post-)Exascale Systems - Part I of II

9:10 AM-10:50 AM

Room:203

For Part 2 see MS115

As computing platforms evolve towards exascale and beyond, resiliency will become a key challenge along with energy consumption, memory access, concurrency and heterogeneous hardware. Both soft and hard fault rates are projected to substantially increase. Programming models and applications will require a resilient infrastructure to be suitable for fault-free simulations over a large number of nodes for reasonable amounts of time. Relying on system and hardware only will not be feasible, and it will be essential for application users to incorporate resilience directly. This minisymposium presents advances addressing resiliency in PDE solvers from both a development and application standpoint.

Organizer: Bert J. Debusschere
Sandia National Laboratories, USA

Organizer: Karla Morris
Sandia National Laboratories, USA

9:10-9:30 Partial Differential Equations Solver Resilient to Soft and Hard Faults

Francesco Rizzi, Karla Morris, and Khachik Sargsyan, Sandia National Laboratories, USA; Paul Mycek and Andres Contreras, Duke University, USA; Cosmin Safta, Sandia National Laboratories, USA; Olivier Le Maitre, LIMSI-CNRS, France; Omar M. Knio, Duke University, USA; *Bert J. Debusschere*, Sandia National Laboratories, USA

9:35-9:55 Building Blocks for Resilient MPI Applications

George Bosilca, University of Tennessee, Knoxville, USA

10:00-10:20 Resilience in the Parareal Method

Jan S. Hesthaven and *Allan Nielsen*, École Polytechnique Fédérale de Lausanne, Switzerland

10:25-10:45 A Soft-Fault Tolerant Advection Solver Via the Sparse Grid Combination Technique

Peter Strazdins, Australian National University, Australia

Tuesday, February 28

MS89

Computational Engineering (BGCE) Student Paper Prize

9:10 AM-10:50 AM

Room:204

For Part 2 see MS116

The 6th Bavarian Graduate School in Computational Engineering (BGCE) Student Paper Prize will be awarded at the 2017 SIAM CSE Conference for outstanding student work in the field of Computational Science and Engineering. Eligible for the prize will be undergraduate and graduate students prior to receiving their PhD. Candidates are required to summarize their work in a short paper of at most 4 pages. The prize finalists will present their work in this minisymposium. The prize award announcement will be scheduled at one of the last days of the conference.

Organizer: Tobias Neckel
Technische Universität München, Germany

Organizer: Michael Rippl
Technische Universität München, Germany

Organizer: Hans-Joachim Bungartz
Technische Universität München, Germany

Organizer: Dietmar Fey
Universität Erlangen-Nürnberg, Germany

Organizer: Alexander Ditter
Universität Erlangen-Nürnberg, Germany

Speakers To Be Announced

Tuesday, February 28

MS90

Approximation of (Parametrized) Eigenvalue Problems - Part I of II

9:10 AM-10:50 AM

Room:205

For Part 2 see MS117

The goal of this minisymposium is to bring together experts working on the approximation of (parametrized) eigenvalue problems. The latter arise in many important applications in science and engineering. Examples are quantum mechanics, the vibro-acoustic analysis of structures, the vibrations of membranes, as well as the response of buildings and bridges to earthquakes and wind. The approximation of eigenvalue problems is (still) challenging for instance because of complex, large-scale geometries or the fact that one is often interested in approximating a certain part of the spectrum at once. We present adaptive Finite Element methods along with recent Isogeometric Analysis. An additional challenge arises from uncertain input data, which leads to parametric eigenvalue problems. The efficient solution of these problems requires the combination of the techniques above with complexity reduction procedures such as Reduced Basis Methods, the Proper Generalized Decomposition approach and Quasi Monte Carlo methods. We demonstrate how those methods can be successfully applied to tackle real-world problems.

Organizer: Thomas Horger
Technische Universität München, Germany

Organizer: Kathrin Smetana
Universität Münster, Germany

Organizer: Elisabeth Ullmann
Technische Universität München, Germany

continued on next page

MS90

Approximation of (Parametrized) Eigenvalue Problems - Part I of II

9:10 AM-10:50 AM

continued

9:10-9:30 Collocation Methods for Exploring Perturbations in Linear Stability Analysis of Dynamical Systems

Howard C. Elman, University of Maryland, College Park, USA; David Silvester, University of Manchester, United Kingdom

9:35-9:55 Applying Quasi-Monte Carlo Integration to a Parameterized Elliptic Eigenvalue Problem

Alexander D. Gilbert, University of New South Wales, Australia

10:00-10:20 Perturbation-Based Reduced Bases for Parametrized Eigenvalue Problems

Virginie Ehrlacher, CERMICS, France; Eric Cancès, École des Ponts ParisTech, France; Damiano Lombardi, Inria Paris-Rocquencourt, France; David Gontier, École Normale Supérieure Paris, France; Antoine Levitt, Inria and Ecole des Ponts ParisTech, France

10:25-10:45 Complexity Reduction for Eigenvalue Problems in Vibro-Acoustics

Thomas Horger, Barbara Wohlmuth, and Linus Wunderlich, Technische Universität München, Germany

Tuesday, February 28

MS91

Recent Advances in Domain Decomposition Methods - Part I of II

9:10 AM-10:50 AM

Room:206

For Part 2 see MS118

With the significant advantages in parallel computation, preconditioning, decoupling multi-physics, etc., domain decomposition methods have become one of the major numerical strategies for solving PDEs. Although great efforts have been made in this area, many practical and analytical challenges remain to be solved. This minisymposium intends to create a forum for researchers to discuss recent advances on these methods for PDEs and how to effectively utilize them to design robust solvers to tackle industrial applications.

Organizer: Yassine Boubendir

New Jersey Institute of Technology, USA

Organizer: Xiaoming He

Missouri University of Science and Technology, USA

9:10-9:30 Effective Transmission Conditions for Domain Decomposition Methods in the Case of the Helmholtz Equation

Yassine Boubendir, New Jersey Institute of Technology, USA

9:35-9:55 Schur Complement Domain Decomposition Methods for the Solution of Multiple Scattering Problems

Catalin Turc, New Jersey Institute of Technology, USA

10:00-10:20 Domain Decomposition for a Mixed Finite Element Method for Linear Elasticity with Weak Symmetry

Eldar Khattatov and Ivan Yotov, University of Pittsburgh, USA

10:25-10:45 A Parareal in Time Algorithm for the Optimal Control of Evolution Equations

Wei Gong, Chinese Academy of Sciences, China

Tuesday, February 28

MS92

Software and Algorithmic Advances for PDE Assembly on Next-generation Architectures - Part I of II

9:10 AM-10:50 AM

Room:209

For Part 2 see MS119

The computing landscape is changing rapidly. To achieve efficient use of next generation architectures in the context of HPC, traditional programming models are being replaced. For example, with the advent of accelerators such as NVIDIA GPUs and Intel PHI, hybrid intranode models such as CUDA and OpenMP are combined with internode MPI. Additionally, the choice in discretization methods such as finite volume, continuous and discontinuous finite elements, and higher order methods may significantly impact scalability and efficiency. This minisymposium highlights the state-of-the-art in algorithms and software for efficient assembly of PDE systems on next generation architectures. The minisymposium will include contributions from applications, PDE frameworks and libraries. Application areas include magnetohydrodynamics/ plasmas, reacting flows, and compressible CFD.

Organizer: Roger Pawlowski

Sandia National Laboratories, USA

Organizer: Eric C. Cyr

Sandia National Laboratories, USA

9:10-9:30 Performance Portable Assembly Tools for Multi-Fluid Plasma Simulation

Roger Pawlowski, Eric C. Cyr, Matthew Bettencourt, Eric Phipps, Christian Trott, H. Carter Edwards, John Shadid, Richard Kramer, and Allen C. Robinson, Sandia National Laboratories, USA

continued on next page

9:35-9:55 Case Studies in Using a DSL and Task Graphs for Portable Reacting Flow Simulations
James C. Sutherland and Tony Saad, University of Utah, USA

10:00-10:20 Efficient High-Order Finite Elements in MFEM
Aaron Fisher, Lawrence Livermore National Laboratory, USA

10:25-10:45 Matrix-Free Operator Evaluation for Finite Element Discretization
Bruno Turcksin, Oak Ridge National Laboratory, USA; Karl Ljungkvist, Uppsala University, Sweden; Martin Kronbichler, Technische Universität München, Germany

Tuesday, February 28

MS93

Advances in Generized Finite Element Methods

9:10 AM-10:50 AM

Room:210

Real-world applications involving multiple materials or physics often lead to the so-caller interface problems. Solution to interface problems involves kinks, discontinuities, singularities, and other non-smooth features. In past decades, many nonstandard finite element methods (FEM) have been developed to solve interface problems efficiently, such as Generalized/ Extended FEM, Nitche's FEM, Immersed FEM. This minisymposium will bring together experts in these fields to discuss recent advances in developing and analyzing nonstandard finite element methods for interface problems.

Organizer: Uday Banerjee
Syracuse University, USA

Organizer: Xu Zhang
Mississippi State University, USA

9:10-9:30 Generalized Finite Element Methods Applied to Interface Problems
Uday Banerjee, Syracuse University, USA; Ivo Babuska, University of Texas at Austin, USA; Qinghui Zhang, Sun Yat-Sen University, China

9:35-9:55 Stable Generalized Finite Element Method for Linear Elastic Fracture Mechanics
Sundararajan Natarajan, Indian Institute of Technology Madras, India

10:00-10:20 Exact Integration Scheme for Planewave-Enriched Partition of Unity Finite Element Method to Solve the Helmholtz Problem
N. Sukumar and Subhajit Banerjee, University of California, Davis, USA

10:25-10:45 A Partition of Unity Method for Generalized Eigenvalue Problems with Application in Electronic Structure Calculations
Marc Alexander Schweitzer, University of Bonn and Fraunhofer SCAI, Germany

Tuesday, February 28

MS94

Parallel-in-Time Integration Methods - Part I of II

9:10 AM-10:50 AM

Room:211

For Part 2 see MS121
New parallel algorithms are required to unlock the computing power provided by massively parallel supercomputers for applications in science and engineering. For the solution of initial value problems, where numerical integration is required along three space and one time dimension, the lack of concurrency in time limits both strong and weak scaling. Parallel-in-time integration methods have been identified as a promising way to increase the level of parallelism in the numerical solution of initial value problems. The minisymposium will collect presentations presenting different aspects and applications of a variety of methods.

Organizer: Daniel Ruprecht
University of Leeds, United Kingdom

Organizer: Robert Speck
Jülich Supercomputing Centre, Germany

9:10-9:30 PFASST and Finite Elements
Robert Speck and Ruth Schoebel, Jülich Supercomputing Centre, Germany; Oliver Sander, Technische Universität Dresden, Germany

9:35-9:55 Toward Space-Time Parallel Climate Simulations Using Pfasst
Andreas Kreienbuehl and Michael Minion, Lawrence Berkeley National Laboratory and Stanford University, USA; Katherine J. Evans, Oak Ridge National Laboratory, USA

10:00-10:20 The Role of Near-Resonance in Parareal Convergence
Adam Peddle and Beth Wingate, University of Exeter, United Kingdom; Terry Haut, Los Alamos National Laboratory, USA

10:25-10:45 On the Time-Parallelization of the Solution of Navier-Stokes Equations Using Parareal
Thibaut Lunet, École nationale supérieure de l'aéronautique et de l'espace; Julien Bodart, École nationale supérieure de l'aéronautique et de l'espace, France; Serge Gratton, ENSEEIHT, Toulouse, France; Xavier Vasseur, CERFACS, France

Tuesday, February 28

MS95

Numerical and Computational Challenges in High Order DG Methods - Part I of II

9:10 AM-10:50 AM

Room:212

For Part 2 see MS122

Discontinuous Galerkin methods have become popular for problems (such as wave propagation and fluid dynamics) where high order schemes are advantageous. However, it can be difficult to maintain robustness, computational efficiency, accuracy, and energy stability when incorporating non-trivial features (e.g., adaptivity, curved elements, couplings to other methods, or absorbing boundaries) into DG solvers. In this minisymposium, we have collected a range of presentations covering recent numerical, mathematical, and computational advances in these areas.

Organizer: Jesse Chan
Rice University, USA

Organizer: Russell Hewett
Total E &P, USA

9:10-9:30 Three Tricks to Tame the CFL in Discontinuous Galerkin Methods

Daniel Appelo, University of New Mexico, USA; Thomas M. Hagstrom, Southern Methodist University, USA; Fengyan Li, Rensselaer Polytechnic Institute, USA; Matt Pennybacker and Adeline Kornelus, University of New Mexico, USA

9:35-9:55 DG Methods on Hybrid Grids for Simulating Waves

Thomas M. Hagstrom, Southern Methodist University, USA; Jeff Banks, Rensselaer Polytechnic Institute, USA; Jeremy E. Kozdon and Lucas Wilcox, Naval Postgraduate School, USA

10:00-10:20 On the Stability of Mesh Adaptivity for Discontinuous Galerkin Methods

Jeremy E. Kozdon and Lucas Wilcox, Naval Postgraduate School, USA

10:25-10:45 Weight-Adjusted Discontinuous Galerkin Methods for Heterogeneous Media and Curvilinear Meshes

Jesse Chan, Rice University, USA; Russell Hewett, Total E&P, USA; Tim Warburton, Virginia Tech, USA

Tuesday, February 28

MS96

Numerical Simulation of Optical and Plasmonic Phenomena - Part I of II

9:10 AM-10:50 AM

Room:213

For Part 2 see MS123

The main purpose of this minisymposium is to bring together specialists in the numerical ?simulation of optical phenomena. Driven by spectacular advances in the design capabilities of materials at the nanoscale, there has been significant recent growth in the field of nano-optics. In particular, algorithm design, analysis, and implementations of mathematical models in the area are now at the heart of everyday technologies. Despite this, some very important issues still remain open. This minisymposium is meant to be a platform to exchange ideas on these problems.

Organizer: Youngjoon Hong
University of Illinois, Chicago, USA

Organizer: David P. Nicholls
University of Illinois, Chicago, USA

9:10-9:30 Inverse Random Source Scattering Problems in Several Dimensions

Peijun Li, Purdue University, USA

9:35-9:55 Nonlinear Photoacoustic Tomography with Two-Photon Absorption

Kui Ren and Rongting Zhang, University of Texas at Austin, USA

10:00-10:20 Spectral Element Simulation for Nanowire Solar Cells on HPC Platforms

MiSun Min, Argonne National Laboratory, USA

10:25-10:45 Scattering and Field Enhancement of Narrow Slits

Junshan Lin, Auburn University, USA

Tuesday, February 28

MS97

Recent Developments in Discontinuous Galerkin Methods - Part I of II

9:10 AM-10:50 AM

Room:214

For Part 2 see MS124

Discontinuous Galerkin (DG) methods have attracted considerable attention in recent years, emerging as a promising approach to solve increasingly complex continuum problems in engineering. This minisymposium explorers recent developments in DG methods including, but not limited to, applications of DG methods to complex aerodynamic flows, analyses of entropy- and energy-stable schemes, developments of error estimation and adaptation techniques, and generalizations of DG framework. We bring together researchers working on both fundamental and applied aspects of DG methods to provide a forum for discussion, interaction, and further development of DG methods.

Organizer: Masayuki Yano
University of Toronto, Canada

Organizer: Cuong Nguyen
Massachusetts Institute of Technology, USA

9:10-9:30 Stage-Parallel Implicit Runga-Kutta Time-Integration and Efficient Approximate Block Preconditioning for Discontinuous Galerkin Methods

Per-Olof Persson, University of California, Berkeley, USA; Will Pazner, Brown University, USA

9:35-9:55 Towards Combined CG-DG for Elliptic Problems

Martin Vymazal and Spencer Sherwin, Imperial College, United Kingdom

continued on next page

10:00-10:20 Metric-Based HP-Adaptation Using a Continuous Mesh Model

Georg May and *Ajay Rangarajan*, RWTH Aachen University, Germany; Vit Dolejsi, Charles University, Czech Republic

10:25-10:45 Energy-Conservative HDG Methods for the Wave Equation

Cuong Nguyen, Massachusetts Institute of Technology, USA; Cristian Ciuca, Imperial College, United Kingdom; Jaime Peraire, Massachusetts Institute of Technology, USA; Bernardo Cockburn, University of Minnesota, Minneapolis, USA

Tuesday, February 28

MS98

Positivity Preserving and Invariant Domain Preserving Methods - Part I of II

9:10 AM-10:50 AM

Room:215

For Part 2 see MS125

Positive density and internal energy are invariant properties for the Euler equations; likewise, positive water height is an invariant property of the shallow water equations. Many first-order methods are known to be invariant-domain preserving, but extending theses techniques to higher-order is non-trivial. The difficulty consists of being invariant, high-order accurate and to satisfy enough entropy inequalities for the approximation to converge to an entropy solution. Invariant-domain preserving are important in applications where being 'in bounds' is essential. The objective of minisymposium is to gather specialists to present the latest developments on invariant-domain preserving methods for the approximation of hyperbolic systems.

Organizer: Bojan Popov

Texas A&M University, USA

Organizer: Xiangxiong Zhang

Purdue University, USA

9:10-9:30 Positivity-Preserving High Order Discontinuous Galerkin Schemes for Compressible Navier-Stokes Equations

Xiangxiong Zhang, Purdue University, USA

9:35-9:55 An Implicit Positivity Preserving Discontinuous Galerkin Method for Solving Conservation Laws

Tong Qin, Brown University, USA

10:00-10:20 On All-Regime and High-Order Lagrange-Remap Numerical Schemes for Compressible Fluids Systems

Christophe Chalons, Versailles Saint-Quentin-en-Yvelines University, France

10:25-10:45 Conservation and Positivity Preserving Issues for Kinetic Collisional Transport Models

Irene M. Gamba, University of Texas at Austin, USA

Tuesday, February 28

MS99

Efficient Numerical Methods for Nonlinear PDE

9:10 AM-10:50 AM

Room:216

The numerical approximation of nonlinear equations poses unique challenges not encountered in linear systems. Nonlinear systems are generally approached by solving a sequence of linear equations; however, the choice of this sequence and how it is solved can greatly impact the convergence properties of the method, including whether it converges to a good approximation of the PDE solution, whether it converges within a reasonable time frame, and if it even converges at all. The goal of the session is to connect a broad range of techniques used to approach these challenging problems, including discretization, regularization, upscaling, and iterative methods. We highlight recent innovations applied to a variety of both steady state and time dependent problems.

Organizer: Sara Pollock

Wright State University, USA

Organizer: Yunrong Zhu

Idaho State University, USA

9:10-9:30 Efficient Simulation of Asymptotically Disappearing Solutions for Wave and Maxwell's Equations

James H. Adler and *Xiaozhe Hu*, Tufts University, USA; Vesselin Petkov, Université Bordeaux I, France; Ludmil Zikatanov, Pennsylvania State University, USA

9:35-9:55 Finite Element Methods for the Stochastic Allen-Cahn Equation with Gradient-Type Multiplicative Noises

Xiaobing H. Feng, University of Tennessee, USA; *Yukun Li*, Ohio State University, USA; Yi Zhang, University of Notre Dame, USA

10:00-10:20 An Efficient Adaptive Grid Method for the Numerical Solution of Phase-Field Models

Mohamed Sulman, Wright State University, USA

10:25-10:45 Gmsfem for a Class of Nonlinear PDEs

Eric Chung, Chinese University of Hong Kong, Hong Kong

Tuesday, February 28

MS100

Numerical Methods for Electronic Structure Calculations: Excited State Properties - Part I of II

9:10 AM-10:50 AM

Room:217

For Part 2 see MS127

This is the second part of two minisymposia on numerical methods for electronic structure calculations. This minisymposium focuses on excited states calculations. Quantitative predictions for excited state phenomena are at the leading edge of modern theories for 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, time dependent density functional theory etc.

Organizer: Chao Yang

Lawrence Berkeley National Laboratory, USA

Organizer: Lin Lin

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

9:10-9:30 Recent Progress on Reducing the Cost of the Fock Exchange Operator

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

9:35-9:55 Electronic Density of States for Incommensurate Layers

Mitchell Luskin, University of Minnesota, USA; Christoph Ortner, University of Warwick, United Kingdom; Daniel Massatt, University of Minnesota, USA

10:00-10:20 Adaptive Quantum Chemistry Methods for Strongly Correlated Electrons with Tunable Accuracy

Francesco Evangelista, Jeffrey Schriber, and Tianyuan Zhang, Emory University, USA

10:25-10:45 Methodological Developments in the Calculation of Excited-State Properties: Large Scale GW Calculations

Marco Govoni, Argonne National Laboratory, USA; Giulia Galli, University of Chicago and Argonne National Laboratory, USA

continued in next column

Tuesday, February 28

MS101

Parallel Numerical Linear Algebra for Extreme Scale Systems

9:10 AM-10:50 AM

Room:218

Today's most powerful supercomputers are composed of hundreds of thousands of computing cores (CPUs and accelerators) connected in high speed networks that make up a massively parallel high performance computing (HPC) system. These systems are placing new demands on effective scalable numerical algorithms and software libraries, which will only increase in the future as we move towards increasingly heterogeneous systems with millions of compute cores. This minisymposium focuses on addressing these challenges in the context of linear algebra problems through developing novel parallel algorithms, exploring advanced scheduling strategies and runtime systems, carrying out offline and online autotuning, and avoiding communication and synchronization bottlenecks.

Organizer: Nicholas J. Higham

University of Manchester, United Kingdom

Organizer: Bo T. Kågström

Umeå University, Sweden

9:10-9:30 The Design and Implementation of a Dense Linear Algebra Library for Extreme Parallel Computers

Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA; Nicholas Higham, University of Manchester, United Kingdom; Zounon Mawussi, Inria, France; Samuel Relton, University of Manchester, United Kingdom

9:35-9:55 Computing the Low Rank Approximation of a Sparse Matrix

Laura Grigori and Sebastien Cayrols, Inria, France; James W. Demmel, University of California, Berkeley, USA; Alan Ayala, Inria, France

continued on next page

10:00-10:20 Sparse Direct Solvers for Extreme Scale Computing

Iain Duff, Science & Technology Facilities Council, United Kingdom and CERFACS, Toulouse, France; Jonathan Hogg, Florent Lopez, and Stojce Nakov, Rutherford Appleton Laboratory, United Kingdom

10:25-10:45 Extreme-Scale Eigenvalue Reordering in the Real Schur Form

Lars Karlsson, *Carl Christian Kjelgaard Mikkelsen*, and Bo T. Kågström, Umeå University, Sweden

Tuesday, February 28

MS102

Modern Eigenvalue Solvers for Applications in Computational Science and Engineering - Part I of II

9:10 AM-10:50 AM

Room:219

For Part 2 see MS129

A common computational task in many scientific computing applications is the solution of one or more eigenvalues problems. The choice of a solver for a specific problem often depends on the properties and structure of the defining matrices: from large and sparse to relatively small and dense, from single problems to sequences of them. This minisymposium addresses the eigenproblems heterogeneity in connection with the rich variety of modern software packages and implementations which are used to solve them. The ultimate goal is to make computational specialists and computer scientists aware of the current status of research and scientific advancement.

Organizer: Edoardo A. Di Napoli
Jülich Supercomputing Centre, Germany

Organizer: Eric Polizzi
University of Massachusetts, Amherst, USA

Organizer: Yousef Saad
University of Minnesota, USA

9:10-9:30 The Chase Library and Its Application to Excitoning Hamiltonians

Edoardo A. Di Napoli, Jülich Supercomputing Centre, Germany; Jan Winkelmann, RWTH Aachen University, Germany; Andre Schleife, University of Illinois at Urbana-Champaign, USA

9:35-9:55 Parallel Rational Arnoldi Algorithm and Applications

Mario Berljafa and Stefan Guettel, University of Manchester, United Kingdom

10:00-10:20 Experiences with GPU Use in Eigenvalue Computations with SLEPc

Jose E. Roman, Universidad Politecnica de Valencia, Spain

10:25-10:45 Applications of the Parallel Complex Moment-Based Eigensolver Package z-Pares to Large-Scale Scientific Computations

Yasunori Futamura, Akira Imakura, and Tetsuya Sakurai, University of Tsukuba, Japan

Tuesday, February 28

MS103

High-Performance Graph Algorithms - Part I of II

9:10 AM-10:50 AM

Room:220

For Part 2 see MS130

Graph algorithms play an important role in the manipulation, distribution and analysis of large data sets arising from both traditional and emerging computational science applications. This minisymposium brings together researchers engaged in developing high-performance parallel graph algorithms with applications to parallel computing, linear system solvers, genomics, neuroscience, and cybersecurity.

Organizer: Karen D. Devine
Sandia National Laboratories, USA

Organizer: Kamesh Madduri
Pennsylvania State University, USA

Organizer: Siva Rajamanickam
Sandia National Laboratories, USA

9:10-9:30 Maintaining Connected Components for Infinite Graph Streams

Jonathan Berry, Sandia National Laboratories, USA; Matthew Oster, Pacific Northwest National Laboratory, USA; *Cynthia Phillips*, Steve Plimpton, and Timothy Shead, Sandia National Laboratories, USA

9:35-9:55 Updating Dynamic Networks in Parallel Using Graph Sparsification

Sanjukta Bhowmick and Sriram Srinivasan, University of Nebraska, Omaha, USA

10:00-10:20 Computing Graph Centrality

Erik Saule, University of North Carolina, Charlotte, USA; A. Erdem Sariyuce, Sandia National Laboratories, USA; Kamer Kaya, Sabanci University, Turkey; Umit V. Catalyurek, Georgia Institute of Technology, USA

10:25-10:45 High-Performance Graph Traversal for De Bruijn Graph-Based Metagenome Assembly

Vasudevan Rengasamy and Kamesh Madduri, Pennsylvania State University, USA

Tuesday, February 28

MS104

Computational Challenges for Heterogeneous Applications on GPU and KNL - Part I of II

9:10 AM-10:50 AM

Room:Crystal AF - 1st Fl

For Part 2 see MS131

Large-scale computing capabilities are on the horizon, opening up new prospects for Computational Sciences. As hardware moves towards heterogeneous systems, application scientists face many computational challenges in order to use them efficiently. We propose a minisymposium to present the view from leading scientists on how to addresses these issues in selected application areas, such as energy, material design, weather prediction, and CFD-modeling. We will start by exploring multicore/GPU-based architectures and runtime improvements, as a generic way to accelerate applications utilizing linear algebra (especially the eigenvalue problems), and then concentrate on specific applications and their respective challenges from academia and industry.

Organizer: Stanimire Tomov

University of Tennessee, Knoxville, USA

9:10-9:30 Implementation of Parallel FFTs on Knights Landing Cluster

Daisuke Takahashi, University of Tsukuba, Japan

9:35-9:55 An Applications Perspective on Multi-Core, Massive Multi-Threading, and Hybrid Systems

Thomas C. Schulthess, ETH Zürich, Switzerland

10:00-10:20 Implementation Techniques for High Performance Blas Kernels on Modern GPUS

Daichi Mukunoki, RIKEN, Japan

10:25-10:45 H Or Not to H: Hierarchical vs Dense Matrix Computations on Manycore Architectures

Kadir Akbudak, Bilkent University, Turkey; Ali Charara, David E. Keyes, *Hatem Ltaief*, and Aleksandr Mikhalev, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; George M Turkiyyah, American University of Beirut, Lebanon

Tuesday, February 28

MS105

Advanced Scientific Computing using Julia - Part I of II

9:10 AM-10:50 AM

Room:Crystal CD - 1st Fl

For Part 2 see MS132

This minisymposium showcases recent developments and applications for advanced scientific computing in Julia. Julia is a dynamic high-level language for technical computing, which is increasingly being used for solving complex and large-scale problems. It is developed and maintained by an large and active group of developers from around the world. This minisymposium brings together a wide range of applications of Julia in network analysis, optimization, inverse problems, partial differential equations, and parallel computing.

Organizer: Lars Ruthotto

Emory University, USA

Organizer: Chen Jiahao

Massachusetts Institute of Technology, USA

9:10-9:30 Krylov Methods with a Forward Error Minimization Property and Application to Optimization

Dominique Orban, École Polytechnique de Montréal, Canada; Ron Estrin and Michael A. Saunders, Stanford University, USA

9:35-9:55 Fast and Memory Efficient Statistical Analysis of Large Genomic Data Sets

Andreas Noack, Massachusetts Institute of Technology, USA

10:00-10:20 Shifted Laplacian Multigrid for the Elastic Helmholtz Equation

Eran Treister, Ben Gurion University Negev, Israel; Eldad Haber, University of British Columbia, Canada

10:25-10:45 Optimal Numerical Methods for Stochastic PDEs

Clemens Heitzinger, Amirreza Khodadadian, and Gudmund Pammer, Vienna University of Technology, Austria; Stefan Rigger, Technische Universität Wien, Austria and Arizona State University, USA; Leila Taghizadeh, Vienna University of Technology, Austria

Tuesday, February 28

MS106

Reduced Order Models for Fluids: Achievements and Open Problems - Part I of II

9:10 AM-10:50 AM

Room:301

For Part 2 see MS133

This minisymposium aims at giving a survey of recent developments in the reduced order modeling of fluid flows. Computational modeling, numerical analysis and applications to realistic engineering and geophysical flow problems will be covered in this minisymposium. Both achievements and open problems in the reduced order modeling of fluid flows will be discussed.

Organizer: Traian Iliescu

Virginia Tech, USA

9:10-9:30 A Multiscale Reduced-Order Model for NS Equations from Residual Minimization

Andrea Ferrero and Michel Bergmann, Inria Bordeaux Sud-Ouest, France; *Angelo Iollo*, Institut de Mathématiques de Bordeaux, France

9:35-9:55 On the use of the Mori-Zwanzig Formalism to Build Closures for Reduced-Order Models

Ayoub Gouasmi and Karthik Duraisamy, University of Michigan, Ann Arbor, USA

10:00-10:20 Large Eddy Simulation Reduced Order Models

Xuping Xie, Virginia Tech, USA

10:25-10:45 Strategies for Modeling Nonlinear Mechanisms from Data

Eurika Kaiser, University of Washington, USA

Tuesday, February 28

MS107

Model Order Reduction: Perspectives from Junior Researchers - Part I of II

9:10 AM-10:50 AM

Room:302

For Part 2 see MS134

The increasing demands on computational models, and their ever-growing complexity made model reduction ubiquitous in many areas of computational science and engineering. By exploiting the structure of mathematical models, impressive reductions in state-dimension can be achieved, while retaining important features of the full dimensional model. In this minisymposium, the next generation of young researchers in model reduction presents a breadth of work on new methods, and exciting applications, such as: fluid dynamics, fire simulations, and transport phenomena.

Organizer: Boris Kramer

Massachusetts Institute of Technology, USA

9:10-9:30 Reduced Order Nonlinear Fire Plume Models

Alan Lattimer, Jensen Hughes, USA; Jeff Borggaard, Virginia Polytechnic Institute & State University, USA; Brian Lattimer, Jensen Hughes, USA

9:35-9:55 Hybrid Discontinuous Galerkin Method for POD

Yangwen Zhang, Missouri University of Science and Technology, USA

10:00-10:20 POD Reduced Order Modeling for Evolution Equations Utilizing Arbitrary Finite Element Discretizations

Carmen Graessle and Michael Hinze, Universitat Hamburg, Germany

10:25-10:45 Model Reduction of Multiple Transport Phenomena: The Shifted Proper Orthogonal Decomposition

Philipp Schulze and Julius Reiss, Technische Universität Berlin, Germany

Tuesday, February 28

MS108

Expanding Computing Science Research through Broader Engagement - Part I of II

9:10 AM-10:50 AM

Room:303

For Part 2 see MS135

The goal of the Broader Engagement program at SIAM CSE17 is to expand the computational science and engineering research community by engaging and supporting students and faculty from nontraditional and underrepresented backgrounds. This minisymposium will describe the Broader Engagement program and will include research presentations from faculty and students participating in the CSE17 Broader Engagement program.

Organizer: Mary Ann E. Leung

Sustainable Horizons Institute, USA

9:10-9:30 Catalying the Normalization of Inclusion through Broader Engagement

Mary Ann E. Leung, Sustainable Horizons Institute, USA

9:35-9:55 Big Compute, Big Data, and Better Drugs

Sally R. Ellingson, University of Kentucky, USA

10:00-10:20 Beyond Docking: Increasing the Accuracy of Virtual Screens

Amir Kucharski, University of Kentucky, USA

10:25-10:45 A Framework for the Evaluation of Data Analyses and Visualization Tools

Samar Swaid, Philander Smith College, USA

Tuesday, February 28

MS109

Computational Poromechanics - Part I of II

9:10 AM-10:50 AM

Room:304

For Part 2 see MS136

Despite their central role in many applications, ranging from petroleum to biomedical engineering, the numerical solutions to the PDEs coupling thermal, flow and mechanical processes in porous media are still a challenging task. For instance, the problem of ill-conditioning may arise from large time- and space-scale contrasts, nonlinear material behaviors, heterogeneity, and anisotropy, with an associated significant computational burden. This minisymposium aims at highlighting the current status of research and the recent advances developed to address the main open issues. These may include novel discretization methods, stabilization techniques, original solution algorithms, and inverse coupled modeling.

Organizer: Massimiliano Ferronato

University of Padova, Italy

Organizer: Jinhyun Choo

Stanford University, USA

9:10-9:30 Hydromechanical Modeling Framework for Two-Scale Porous Media

Jinhyun Choo and Ronaldo I. Borja, Stanford University, USA

9:35-9:55 About the Uzawa Smoother for Poroelastic Problems

Francisco José Gaspar, University of Zaragoza, Spain

10:00-10:20 Computation and Joint Analysis of Coupled Flow, Geomechanics, and Geophysics in Reservoir Engineering

Jihoon Kim, Texas A&M University, USA; Evan Um, Lawrence Berkeley National Laboratory, USA

10:25-10:45 Preconditioning Strategies for Coupled Multiphase Poromechanics

Joshua A. White, Lawrence Livermore National Laboratory, USA; Sergey Klevtsov, Nicola Castelletto, and Hamdi Tchelepi, Stanford University, USA

Tuesday, February 28

MS110

Data-Driven Characterization, Control, and Uncertainty Quantification of Dynamical Systems - Part I of II

9:10 AM-10:50 AM

Room:305

For Part 2 see MS137

Data-driven methods play an increasingly vital role across the physical, engineering and biological sciences. The characterization of dynamical systems from data is an especially vibrant field, with solid theoretical and algorithmic underpinnings and applications to control and uncertainty management in real-world systems. This minisymposium brings together experts working at the forefront of data-driven methods, which include techniques from machine learning, compressed sensing, dimension reduction, uncertainty quantification, and control. Topics of interest include sensor placement, nonlinear system identification, model selection, and machine learning for control, with diverse applications to the study of flight dynamics, climate systems, epidemiological models, biological regulatory networks, and turbulence.

Organizer: Travis Askham

University of Washington, USA

Organizer: Eurika Kaiser

University of Washington, USA

9:10-9:30 The Most Informative Data for the State, Parameters and Dynamical Model

Pierre F. Lermusiaux and Jing Lin, Massachusetts Institute of Technology, USA

9:35-9:55 Network Representation and Analysis of Bluff Body Wake

Muralikrishnan Gopalakrishnan Meena, Aditya G. Nair, and Kunihiko Taira, Florida State University, USA

continued in next column

10:00-10:20 Sensor Placement for Multiscale Phenomena

Krithika Manohar, Eurika Kaiser, Steven Brunton, and Nathan Kutz, University of Washington, USA

10:25-10:45 An Extension of the Dynamic Mode Decomposition and Applications

Travis Askham, University of Washington, USA

Tuesday, February 28

MS111

Mixed-Integer PDE Constrained Optimization

9:10 AM-10:50 AM

Room:221

Many complex science and engineering applications can be formulated as optimization problems, constrained by partial differential equations (PDEs), that involve both continuous and integer variables. This class of problems has a broad range of science and engineering applications, including the positioning of wells in ground-water flow, topology optimization, and the design and control of gas networks. This minisymposium introduces the challenges arising from this mixtures of discrete decisions with PDE constraints, highlights new applications, and presents computational solution approaches for this new class of challenging optimization problems.

Organizer: Sven Leyffer

Argonne National Laboratory, USA

9:10-9:30 Discrete Material Optimization of Nano-Structures in Electromagnetic Applications

Michael Stingl, Universität Erlangen-Nürnberg, Germany

9:35-9:55 Mixed-Integer PDE-Constrained Optimization for Gas Networks

Mirko Hahn, Argonne National Laboratory, USA

10:00-10:20 TAO: Toolkit for Advanced Optimization

Todd Munson, Argonne National Laboratory, USA

10:25-10:45 Nonlinear Robust PDE Constrained Optimization Using Approximation Techniques and Model Order Reduction with Application to Electric Motor Design

Oliver Lass and Stefan Ulbrich, Technische Universität Darmstadt, Germany

Tuesday, February 28

MS112

Uncertainty Quantification in Turbulent Flow Simulations - Part I of II

9:10 AM-10:25 AM

Room:222

For Part 2 see MS139

Accurate predictions of turbulent flows are of crucial importance for the design and operation of complex systems such as aircrafts and gas turbine engines. However, it remains challenging to simulate these flows computationally and to estimate system performance with confidence. Prediction uncertainties can emerge from a number of sources, e.g., geometric variability, boundary and initial conditions, and assumptions embedded in engineering models of turbulent motion. This minisymposium aims to bring together researchers working on uncertainty quantification in turbulence modeling and simulations, including (1) input uncertainty, model-from uncertainty, and their coupling, and (2) uncertainties in turbulence modeling approaches of various fidelities.

Organizer: Heng Xiao
Virginia Tech, USA

Organizer: Gianluca Iaccarino
Stanford University, USA

9:10-9:30 A Data-Driven, Physics-Informed Approach for Turbulence Modeling
Heng Xiao, Jinlong Wu, and Jianxun Wang, Virginia Tech, USA

9:35-9:55 A Model Transport Equation for Epistemic UQ in RANS
Wouter N. Edeling and Gianluca Iaccarino, Stanford University, USA; Paola Cinnella, Arts et Métiers ParisTech and Univesità del Salento, France

10:00-10:20 Data-Driven Predictive Modeling of RANS Model Discrepancies
Anand Pratap Singh, University of Michigan, USA; Karthik Duraisamy, University of Michigan, Ann Arbor, USA

Tuesday, February 28

CP7

Uncertainty Quantification - Part I of IV

9:10 AM-10:50 AM

Room:223

For Part 2 see CP9
Chair: To Be Determined

9:10-9:20 Adjoint-Enabled Optimization and UQ for Radiation Shield Design
Brian M. Adams, Sandia National Laboratories, USA

9:22-9:32 Interpolatory Model Reduction of Parameterized Bilinear Dynamical Systems
Andrea Carracedo Rodriguez and Serkan Gugercin, Virginia Tech, USA

9:34-9:44 Ensemble Kalman Filtering for Inverse Optimal Control
Andrea Arnold and Hien Tran, North Carolina State University, USA

9:46-9:56 A Computational Bayesian Framework to Parallelize an Adaptive Markov Chain Monte Carlo
Yasser Soltanpour and Zenon Medina-Cetina, Texas A&M University, USA

9:58-10:08 An Asymptotic-Preserving Stochastic Galerkin Method for the Semiconductor Boltzmann Equation with Random Inputs and Diffusive Scalings
Liu Liu, University of Wisconsin, Madison, USA

10:10-10:20 Stochastic Dirichlet Boundary Optimal Control of Steady Navier-Stokes Equations
Wenju Zhao and Max Gunzburger, Florida State University, USA

10:22-10:32 Bayesian Model Reduction for Nonlinear Dynamics Using Automatic Relevance Determination
Abhijit Sarkar and *Rimple Sandhu*, Carleton University, Canada; Chris Pettit, United States Naval Academy, USA; Mohammad Khalil, Sandia National Laboratories, USA; Dominique Poirel, Royal Military College, Canada

10:34-10:44 Domain Decomposition Algorithms for Uncertainty Quantification: High-Dimensional Stochastic Systems
Abhijit Sarkar and *Ajit Desai*, Carleton University, Canada; Mohammad Khalil, Sandia National Laboratories, USA; Chris Pettit, United States Naval Academy, USA; Dominique Poirel, Royal Military College, Canada

Tuesday, February 28

CP8

Numerical PDEs - Part I of VI

9:10 AM-10:50 AM

Room:224

For Part 2 see CP10
Chair: To Be Determined

9:10-9:20 Mesh Imprinting Reduction by Multi-Dimensional Slope Limiters in Hydrodynamic Simulations
Jan Velechovsky, Marianne M. Francois, and Thomas Masser, Los Alamos National Laboratory, USA

9:22-9:32 Concept of Spectral Differentiation for Solving Corner Flow
Badr Alkahtani, King Saud University, Saudia Arabia

9:34-9:44 Optimal Recovery of Integral Operators and Its Applications
Yuliya Babenko, Kennesaw State University, USA; Vladyslav Babenko, Dnipropetrovsk State University, Ukraine; Natalia Parfinovych and Dmytro Skorokhodov, Oles Honchar Dnipropetrovsk National University, Ukraine

9:46-9:56 A High Order Accurate Direct Solution Technique for High Frequency Problems with Body Loads
Peter Geldermans and Adrianna Gillman, Rice University, USA

9:58-10:08 Compact Implicit Integration Factor Method for Solving High Order Differential Equations
Sameed Ahmed and Xinfeng Liu, University of South Carolina, USA

10:10-10:20 An Optimal Complexity Spectral Method for Elliptic PDEs on Rectangular Domains
Dan Fortunato, Harvard University, USA; Alex Townsend, Cornell University, USA

10:22-10:32 Compatible-Strain Mixed Finite Element Methods for Nonlinear Elasticity
Mostafa Faghih Shojaei and Arash Yavari, Georgia Institute of Technology, USA; Arzhang Angoshtari, George Washington University, USA

10:34-10:44 Scalable Simulation of Systems of PDEs for Modeling Tumor Growth
Elyse Garon and James V. Lambers, University of Southern Mississippi, USA

Tuesday, February 28

Coffee Break

10:50 AM-11:20 AM

Room:Foyer - 2nd Fl

IP4

Making Sense of our Universe with Supercomputers

11:20 AM-12:05 PM

Room:Grand Ballroom - 2nd Fl

Chair: Clint Dawson, University of Texas at Austin, USA

In computational cosmology and astrophysics we encounter some of the most complex multi-scale and multi-physics problems. In the past decades, algorithmic advances have enabled ever more realistic numerical models of a very wide range of astrophysical objects. These range from stars to galaxies, from planets to the large scale structure of the Universe, from molecular clouds to star clusters, from supernovae explosions to super-massive black holes in centers of galaxies. We routinely create three dimensional models of how our Universe may have originated, how its structure formed, how the very first stars and galaxies came about, how pulsars work, and how black holes merge and generate gravitational waves to just name a few such applications. We will highlight some examples of three particular algorithmic breakthroughs and the particular advances and insights they have enabled so far. These describe adaptive mesh refinement simulations capturing 15 orders of magnitude in length scale, adaptive ray tracing for high accuracy radiation hydrodynamical simulations, as well as a new noise-free approach to solve the collisionless Boltzmann equation of interest in cosmology as well as in plasma physics. We will also present the scientific visualizations created from these simulations. These have been shown on various television programs, international planetarium shows and numerous print media.

Tom Abel

Stanford University, USA

Tuesday, February 28

Lunch Break

12:05 PM-1:30 PM

Attendees on their own

PD2

Funding Panel

12:15 PM-1:30 PM

Room:Ballroom D - 2nd Fl

Chair: Youssef M. Marzouk, Massachusetts Institute of Technology, USA

Chair: Hans De Sterck, University of Waterloo, Canada

What opportunities are available for obtaining research funding? What makes a research proposal stand out? How can you build a research program that is attractive to the funding agencies? How can you conduct your research to make the biggest impact and increase your chances of future funding? We address all these questions and more as a part of this panel discussion.

Jean-Luc Cambier
Air Force Research Laboratory, USA

Sinnou David
CNRS, France

Iain Duff
Science & Technology Facilities Council, United Kingdom and CERFACS, Toulouse, France

Fariba Fahroo
Air Force Office of Scientific Research, USA

Abani Patra
State University of New York, Buffalo, USA

Ssushil Prasad
National Science Foundation, USA

Tuesday, February 28

MT4

CSE Collaboration through Software: Improving Productivity and Sustainability- Part II

1:30 PM-3:10 PM

Room:Ballroom C - 2nd Fl

For Part 1 see MT3

Chair: Lois Curfman McInnes, Argonne National Laboratory, USA

CSE software—crosscutting technology that connects advances in mathematics, computer science, and domain-specific science and engineering—is a foundation of sustained CSE collaboration and scientific progress. However, the need for increasingly broad functionality on ever more complex computer architectures creates daunting challenges for software development and sustainability. This tutorial will provide information on best practices in software engineering explicitly tailored for CSE. Goals are improving the productivity of those who develop CSE software and increasing the sustainability of software artifacts. We will discuss practices that are relevant for projects of all sizes, with emphasis on small teams (for example, a faculty member and collaborating students). Part 1: Why effective software practices are essential for CSE projects; understanding what you want from your CSE software and how to achieve it; software testing; integrated software lifecycle. Part 2: Software licensing; effective models, tools, processes, and practices for small software teams; how to collaborate (around code) with people outside your domain; agile workflow management for small teams. Target attendees include CSE investigators who develop software and people who plan and fund CSE projects that incorporate software. The tutorial will incorporate interactive exercises, including a walk through of small team and agile activities for an example GitHub project.

continued on next page

Speakers:

Lois Curfman McInnes
Argonne National Laboratory, USA

David E. Bernholdt
Oak Ridge National Laboratory, USA

Anshu Dubey
Argonne National Laboratory, USA

Michael Heroux
Sandia National Laboratories, USA

Alicia Klinvex
Sandia National Laboratories, USA

Tuesday, February 28

MS113

Coupling Methods in Multiphysics and Multiscale Problems - Part II of II

1:30 PM-2:45 PM

Room:Grand Ballroom - 2nd Fl

For Part 1 see MS85

There has been great interests in the computational methods for multiphysics and multiscale problems due to their importance in engineering and biomedical applications. In the numerical algorithms, information needs to be exchanged at the interface, which brings nonlinearities into the coupled system. Therefore, tackling the immanent complexity of interface and coupling strategies requires crossdisciplinary thinking, sophisticated modeling and advanced numerical methods. This minisymposium will focus on the advanced coupling strategies for multiphysics and multiscale problems. It aims at bringing together researchers from across the applied mathematics and engineering communities to discuss and exchange new ideas for developing efficient and reliable coupling algorithms, and to transfer knowledge between the two communities. Topics of interest include, but not limited to, stabilized methods for coupling frameworks, novel numerical methods for fluid-structure interaction, algorithmic aspects in biomechanics simulations, coupling between local and nonlocal models, and the complex dynamics of molecular biosciences.

Organizer: Yue Yu
Lehigh University, USA

Organizer: Xingjie Li
University of North Carolina, Charlotte, USA

continued in next column

1:30-1:50 A New Predictor-Corrector Method for Efficient Modeling of Surface Effects

Andrew Binder, University of Minnesota, Twin Cities, USA; Mitchell Luskin, University of Minnesota, USA; Christoph Ortner, University of Warwick, United Kingdom

1:55-2:15 Three-Dimensional Elasto-Plastic Simulation of Bulk Metallic Glasses

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

2:20-2:40 Simulations of Viscous Suspension Flows with a Meshless MLS Scheme

Amanda Howard, Brown University, USA; Nathaniel Trask, Sandia National Laboratories, USA; Martin Maxey, Brown University, USA

Tuesday, February 28

MS114

Partial Differential Equation Techniques for Network Problems - Part II of II

1:30 PM-3:10 PM

Room:202

For Part 1 see MS87

Network problems are prevalent in image processing and data analysis, for example in image segmentation, data classification, and community detection. In recent years new approaches to such problems have been proposed, based on techniques from partial differential equations and variational methods. These approaches offer new possibilities for computationally feasible applications to large data sets, as well as exciting new theoretical connections between partial differential equations and applied analysis on the one hand and network science and graph theory on the other. This minisymposium will bring together scientists from the US and Europe who are working on both the computational and theoretical aspects of the field.

Organizer: Yves van Gennip

University of Nottingham, United Kingdom

Organizer: Carola Schönlieb

University of Cambridge, United Kingdom

1:30-1:50 Error Estimates on Spectral Convergence of Graph Laplacian Towards the Laplace-Beltrami Operator

Nicolas Garcia Trillos, Carnegie Mellon University, USA; Moritz Gerlach, Universität Potsdam, Germany; Matthias Hein, Saarland University, Germany; *Dejan Slepcev*, Carnegie Mellon University, USA

1:55-2:15 Generalized Convolutional Representation for Field Data on Graphs

Cristina Garcia-Cardona, Los Alamos National Laboratory, USA

2:20-2:40 Applications of the Graph P-Laplacian for Data Processing and Analysis

Daniel Tenbrinck, Universität Münster, Germany

2:45-3:05 Consistency of Dirichlet Partitions

Braxton Osting and Todd Reeb, University of Utah, USA

Tuesday, February 28

MS115

Resilient PDE Solvers for (Post-)Exascale Systems - Part II of II

1:30 PM-3:10 PM

Room:203

For Part 1 see MS88

As computing platforms evolve towards exascale and beyond, resiliency will become a key challenge along with energy consumption, memory access, concurrency and heterogeneous hardware. Both soft and hard fault rates are projected to substantially increase. Programming models and applications will require a resilient infrastructure to be suitable for fault-free simulations over a large number of nodes for reasonable amounts of time. Relying on system and hardware only will not be feasible, and it will be essential for application users to incorporate resilience directly. This minisymposium presents advances addressing resiliency in PDE solvers from both a development and application standpoint.

Organizer: Bert J. Debusschere

Sandia National Laboratories, USA

Organizer: Karla Morris

Sandia National Laboratories, USA

1:30-1:50 A Fault-Tolerant Implementation of the TeaLeaf Cg Sparse Iterative Solver

Simon McIntosh-Smith, University of Bristol, United Kingdom

1:55-2:15 Local Recovery of Hybrid Task-Parallel Explicit PDE Solvers from Hard Failures

Keita Teranishi and Nicole Slattengren, Sandia National Laboratories, USA

continued in next column

2:20-2:40 Resilience Without Recovery in Algorithms for Hyperbolic Conservation Laws

Jeffrey A. Hittinger and John Loffeld, Lawrence Livermore National Laboratory, USA

2:45-3:05 Acceleration of Monte Carlo Methods for Stochastic Elliptic PDEs Using Domain Decomposition and PC Approximations of Local Dirichlet Maps

Andres Contreras and Paul Mycek, Duke University, USA; Olivier Le Maitre, LIMSI-CNRS, France; Francesco Rizzi, Karla Morris, Khachik Sargsyan, Cosmin Safta, and Bert J. Debusschere, Sandia National Laboratories, USA; Omar M. Knio, Duke University, USA

Tuesday, February 28

MS116

Computational Engineering (BGCE) Student Paper Prize

1:30 PM-3:10 PM

Room:204

For Part 1 see MS89

The 6th Bavarian Graduate School in Computational Engineering (BGCE) Student Paper Prize will be awarded at the 2017 SIAM CS&E Conference for outstanding student work in the field of Computational Science and Engineering. Eligible for the prize will be undergraduate and graduate students prior to receiving their PhD. Candidates are required to summarize their work in a short paper of at most 4 pages. The prize finalists will present their work in this minisymposium. The prize award announcement will be scheduled at one of the last days of the conference.

Organizer: Tobias Neckel
Technische Universität München, Germany

Organizer: Michael Rippl
Technische Universität München, Germany

Organizer: Hans-Joachim Bungartz
Technische Universität München, Germany

Organizer: Dietmar Fey
Universität Erlangen-Nürnberg, Germany

Organizer: Alexander Ditter
Universität Erlangen-Nürnberg, Germany

Speakers To Be Announced

Tuesday, February 28

MS117

Approximation of (Parametrized) Eigenvalue Problems - Part II of II

1:30 PM-3:10 PM

Room:205

For Part 1 see MS90

The goal of this minisymposium is to bring together experts working on the approximation of (parametrized) eigenvalue problems. The latter arise in many important applications in science and engineering. Examples are quantum mechanics, the vibro-acoustic analysis of structures, the vibrations of membranes, as well as the response of buildings and bridges to earthquakes and wind. The approximation of eigenvalue problems is (still) challenging for instance because of complex, large- scale geometries or the fact that one is often interested in approximating a certain part of the spectrum at once. We present adaptive Finite Element methods along with recent Isogeometric Analysis. An additional challenge arises from uncertain input data, which leads to parametric eigenvalue problems. The efficient solution of these problems requires the combination of the techniques above with complexity reduction procedures such as Reduced Basis Methods, the Proper Generalized Decomposition approach and Quasi Monte Carlo methods. We demonstrate how those methods can be successfully applied to tackle real-world problems.

Organizer: Thomas Horger
Technische Universität München, Germany

Organizer: Kathrin Smetana
Universität Münster, Germany

Organizer: Elisabeth Ullmann
Technische Universität München, Germany

continued in next column

1:30-1:50 The Spectral Projector for Eigenvalue/Vector Approximation and Error Estimation

Jeffrey S. Ovall and Jay Gopalakrishnan, Portland State University, USA; Luka Grubisic, University of Zagreb, Croatia

1:55-2:15 Flexible Eigensolvers in Electronic Structure Calculations

Agnieszka Miedlar, University of Kansas, USA; Yousef Saad, University of Minnesota, USA

2:20-2:40 Shape Optimization in Spectral Geometry: A Bayesian Approach

Sebastian Dominguez and Nilima Nigam, Simon Fraser University, Canada; Bobak Shahriari, University of British Columbia, Canada

2:45-3:05 Finite Element Approximation of Eigenvalue Clusters of the Laplace-Beltrami Operator

Justin Owen, Texas A&M University, USA

Tuesday, February 28

MS118

Recent Advances in Domain Decomposition Methods - Part II of II

1:30 PM-3:10 PM

Room:206

For Part 1 see MS91

With the significant advantages in parallel computation, preconditioning, decoupling multi-physics, etc., domain decomposition methods have become one of the major numerical strategies for solving PDEs. Although great efforts have been made in this area, many practical and analytical challenges remain to be solved. This minisymposium intends to create a forum for researchers to discuss recent advances on these methods for PDEs and how to effectively utilize them to design robust solvers to tackle industrial applications.

Organizer: Yassine Boubendir

New Jersey Institute of Technology, USA

Organizer: Xiaoming He

Missouri University of Science and Technology, USA

1:30-1:50 Domain Decomposition in the Wave Chaos Analysis

Zhen Peng, University of New Mexico, USA

1:55-2:15 A Domain Decomposition Based Method for the Simulation of Wind Flows Over Large Urban Areas

Zhengzheng Yan, Shenzhen Institute of Advanced Technology, China; Xiao-Chuan Cai, University of Colorado Boulder, USA; *Rongliang Chen*, Chinese Academy of Sciences, China

2:20-2:40 Robust CFD Algorithms Through On-Line Machine-Learning: Gaussian Process Regression and Diffusion Maps

Seungjoon Lee, Brown University, USA; Ioannis Kevrekidis, Princeton University, USA; George Em Karniadakis, Brown University, USA

2:45-3:05 A Multi-Physics Domain Decomposition Method for Navier-Stokes-Darcy Model

Changxin Qiu, Missouri University of Science and Technology, USA

Tuesday, February 28

MS119

Software and Algorithmic Advances for PDE Assembly on Next-generation Architectures - Part II of II

1:30 PM-3:10 PM

Room:209

For Part 1 see MS92

The computing landscape is changing rapidly. To achieve efficient use of next generation architectures in the context of HPC, traditional programming models are being replaced. For example, with the advent of accelerators such as NVIDIA GPUs and Intel PHI, hybrid intranode models such as CUDA and OpenMP are combined with internode MPI. Additionally, the choice in discretization methods such as finite volume, continuous and discontinuous finite elements, and higher order methods may significantly impact scalability and efficiency. This minisymposium highlights the state-of-the-art in algorithms and software for efficient assembly of PDE systems on next generation architectures. The minisymposium will include contributions from applications, PDE frameworks and libraries. Application areas include magnetohydrodynamics/plasmas, reacting flows, and compressible CFD.

Organizer: Roger Pawlowski

Sandia National Laboratories, USA

Organizer: Eric C. Cyr

Sandia National Laboratories, USA

1:30-1:50 Multilevel Parallelism for SU/PG Discretization Within HPCMP Create(™)-AV COFFE for Compressible Rans Equations on Fully Tetrahedral Meshes

Ryan S. Glasby, Jon Erwin, Stephen Wood, and Douglas Stefanski, University of Tennessee, USA; Steve Karman, Pointwise, Inc., USA

1:55-2:15 Performance Portable Software for High Fidelity Simulation of Reacting Flows Using Kokkos Array Abstractions

Ramanan Sankaran, Oak Ridge National Laboratory, USA; Swapnil Desai, University of Tennessee, Knoxville, USA; Bok Jik Lee, Xiao Xu, Francisco E. Hernández Pérez, and Hong G. Im, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

2:20-2:40 Intrepid2: Performance Portable Finite Element Discretization Library

Kyungjoo Kim, Sandia National Laboratories, USA

2:45-3:05 Model-based Performance Optimization for GPU DG-FEM

James Stevens and Andreas Kloeckner, University of Illinois, USA

continued in next column

Tuesday, February 28

MS121

Parallel-in-Time Integration Methods - Part II of II

1:30 PM-3:10 PM

Room:211

For Part 1 see MS94

New parallel algorithms are required to unlock the computing power provided by massively parallel supercomputers for applications in science and engineering. For the solution of initial value problems, where numerical integration is required along three space and one time dimension, the lack of concurrency in time limits both strong and weak scaling. Parallel-in-time integration methods have been identified as a promising way to increase the level of parallelism in the numerical solution of initial value problems. The minisymposium will collect presentations presenting different aspects and applications of a variety of methods.

Organizer: Daniel Ruprecht

University of Leeds, United Kingdom

Organizer: Robert Speck

Jülich Supercomputing Centre, Germany

1:30-1:50 Parareal for Hyperbolic Problems

Allan Nielsen and J*an S. Hesthaven*, École Polytechnique Fédérale de Lausanne, Switzerland

1:55-2:15 Solving Time-Periodic Navier-Stokes Problems Using Spectral Discretization in Time

Daniel Hupp and Peter Arbenz, ETH Zürich, Switzerland; Dominik Obrist, University of Bern, Switzerland

2:20-2:40 ParaExp using Leap-Frog as Integrator for High-Frequency Electromagnetic Simulations

Melina Merkel, *Innocent Niyonzima*, and Sebastian Schöps, Technische Universität Darmstadt, Germany

2:45-3:05 A Posteriori Error Analysis of the Parareal Algorithm

Jehanzeb H. Chaudhry, University of New Mexico, USA; Don Estep and Simon Tavener, Colorado State University, USA

Tuesday, February 28

MS122

Numerical and Computational Challenges in High Order DG Methods - Part II of II

1:30 PM-3:10 PM

Room:212

For Part 1 see MS95

Discontinuous Galerkin methods have become popular for problems (such as wave propagation and fluid dynamics) where high order schemes are advantageous. However, it can be difficult to maintain robustness, computational efficiency, accuracy, and energy stability when incorporating non-trivial features (e.g., adaptivity, curved elements, couplings to other methods, or absorbing boundaries) into DG solvers. In this minisymposium, we have collected a range of presentations covering recent numerical, mathematical, and computational advances in these areas.

Organizer: Jesse Chan

Rice University, USA

Organizer: Russell Hewett

Total E &P, USA

1:30-1:50 A Characteristic-Based CFL Condition for the Discontinuous Galerkin Method on Triangular Meshes

Lilia Krivodonova, University of Waterloo, Canada

1:55-2:15 Splitform Discontinuous Galerkin Methods for the Compressible Navier-Stokes Equations

Gregor Gassner and Andrew R. Winters, University of Cologne, Germany; David A. Kopriva, Florida State University, USA

2:20-2:40 High-Order Absorbing Boundary Conditions for Time-Domain Wave Propagation with DG Methods

Axel Modave, CNRS, France; Andreas Atle, Total E&P, USA; Jesse Chan, Rice University, USA; Russell Hewett, Total E&P, USA; Tim Warburton, Virginia Tech, USA

2:45-3:05 Accelerating Discontinuous Galerkin Methods

Tim Warburton, Virginia Tech, USA; Jesse Chan, Rice University, USA; Gregor Gassner, University of Cologne, Germany; Axel Modave, CNRS, France; Zheng Wang, Rice University, USA; Lucas Wilcox, Naval Postgraduate School, USA

continued in next column

Tuesday, February 28

MS123

Numerical Simulation of Optical and Plasmonic Phenomena

1:30 PM-3:10 PM

Room:213

For Part 1 see MS96

The main purpose of this minisymposium is to bring together specialists in the numerical ?simulation of optical phenomena. Driven by spectacular advances in the design capabilities of materials at the nanoscale, there has been significant recent growth in the field of nano-optics. In particular, algorithm design, analysis, and implementations of mathematical models in the area are now at the heart of everyday technologies. Despite this, some very important issues still remain open. This minisymposium is meant to be a platform to exchange ideas on these problems.

Organizer: Youngjoon Hong

University of Illinois, Chicago, USA

Organizer: David P. Nicholls

University of Illinois, Chicago, USA

1:30-1:50 An Asymptotic Model for Diffraction by Shallow Gratings

Peter B. Monk, University of Delaware, USA

1:55-2:15 A Multi-Scale Model for Optical Responses of Nano-Structures

Gang Bao, Zhejiang University, China; Di Liu, Michigan State University, USA; *Songting Luo*, Iowa State University, USA

2:20-2:40 Minimizing Eigenvalues for Inhomogeneous Rods and Plates

Weitao Chen, University of California, Irvine, USA; Ching-Shan Chou, The Ohio State University, USA; *Chiu-Yen Kao,* Claremont McKenna College, USA

2:45-3:05 Hybrid Inverse Problem for Porous Media

Carlos Perez-Arancibia, Massachusetts Institute of Technology, USA

Tuesday, February 28

MS124

Recent Developments in Discontinuous Galerkin Methods - Part II of II

1:30 PM-3:10 PM

Room:214

For Part 1 see MS97

Discontinuous Galerkin (DG) methods have attracted considerable attention in recent years, emerging as a promising approach to solve increasingly complex continuum problems in engineering. This minisymposium explores recent developments in DG methods including, but not limited to, the application of DG methods to complex aerodynamic flows, the analysis of entropy- and energy-stable schemes, the development of error estimation and adaptation techniques, and the generalization of DG methods. We bring together researchers working on both fundamental and applied aspects of DG methods to provide a forum for discussion, interaction, and further development of DG methods.

Organizer: Masayuki Yano

University of Toronto, Canada

Organizer: Cuong Nguyen

Massachusetts Institute of Technology, USA

1:30-1:50 The Hybridized Discontinuous Galerkin Methods for Large Eddy Simulation

Pablo Fernandez, Cuong Nguyen, and J*aime Peraire*, Massachusetts Institute of Technology, USA

1:55-2:15 An H-P Adaptive Discontinuous Galerkin Method for Unsteady Flows

Johann Dahm and Krzysztof Fidkowski, University of Michigan, USA

2:20-2:40 Estimation, Localization, and Modeling of Output Errors for Higher-Order Galerkin Finite Element Methods

Hugh Carson, David l. Darmofal, Steven R. Allmaras, and Marshall Galbraith, Massachusetts Institute of Technology, USA

2:45-3:05 An Adaptive Discontinuous Galerkin Reduced Basis Element Method

Masayuki Yano, University of Toronto, Canada

Tuesday, February 28

MS125

Positivity Preserving and Invariant Domain Preserving Methods - Part II of II

1:30 PM-3:10 PM

Room:215

For Part 1 see MS98

Positive density and internal energy are invariant properties for the Euler equations; likewise, positive water height is an invariant property of the shallow water equations. Many first-order methods are known to be invariant-domain preserving, but extending theses techniques to higher-order is non-trivial. The difficulty consists of being invariant, high-order accurate and to satisfy enough entropy inequalities for the approximation to converge to an entropy solution. Invariant-domain preserving are important in application where being 'in bounds' is essential. The objective of minisymposium is to gather specialists to present the latest developments on invariant-domain preserving methods for the approximation of hyperbolic systems.

Organizer: Bojan Popov

Texas A&M University, USA

Organizer: Xiangxiong Zhang

Purdue University, USA

1:30-1:50 Well-Balanced Positivity-Preserving Central-Upwind Schemes for Shallow Water Models

Alexander Kurganov, Tulane University, USA

1:55-2:15 Well-Balanced Central-Upwind Schemes for the Euler Equations with Gravitation

Alina Chertock, North Carolina State University, USA

2:20-2:40 Bound Preserving Flux Limiters and Total Variation Stability for High Order Conservative Schemes

Zhengfu Xu, Michigan Technological University, USA

2:45-3:05 On Positivity of Density and Pressure for Finite Volume Methods Based on Relaxation Riemann Solvers for the Compressible Euler Equations

Christian Klingenberg, Wurzburg University, Germany

Tuesday, February 28

MS126

Numerical Methods in Micromagnetics

1:30 PM-2:45 PM

Room:216

Micromagnetics studies magnetic behavior of ferromagnetic materials at sub-micrometer length scales. These scales are large enough to use a continuum PDE model and are small enough to resolve important magnetic structures such as domain walls, vortices and skyrmions. The dynamics of the magnetic distribution in a ferromagnetic material is governed by the Landau-Lifshitz (LL) equation. The equation is highly nonlinear with a non-convex constraint, has several equivalent forms, such as the Landau-Lifshitz-Gilbert equation, and may require solution of an auxiliary problem in the infinite domain on each time step. These impose interesting challenges in the development and analysis in numerical methods and lead to a large family of algorithms. This minisymposium will discuss the latest results and challenges in traditional and new numerical methods for micromagnetics.

Organizer: Eugenia Kim

University of California, Berkeley, USA

Organizer: Konstantin Lipnikov

Los Alamos National Laboratory, USA

1:30-1:50 The Mimetic Finite Difference Method for the Landau-Lifshitz Equation

Eugenia Kim, University of California, Berkeley, USA

1:55-2:15 Optimal Error Estimates of a Linearized Backward Euler FEM for the Landau-Lifshitz Equation

Huadong Gao, Huazhong University of Science & Technology, China

2:20-2:40 A Self-Consistent Spin-Diffusion Model for Micromagnetics: Discretization and Boundary Conditions

Claas Abert, Technische Universitaet Wien, Austria

Tuesday, February 28

MS127

Numerical Methods for Electronic Structure Calculations: Excited State Properties - Part II of II

1:30 PM-2:45 PM

Room:217

For Part 1 see MS100

This is the second part of two minisymposia on numerical methods for electronic structure calculations. This minisymposium focuses on excited states calculations. Quantitative predictions for excited state phenomena are at the leading edge of modern theories for 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, time dependent density functional theory etc.

Organizer: Chao Yang

Lawrence Berkeley National Laboratory, USA

Organizer: Lin Lin

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

1:30-1:50 Recent Progress in Numerical Methods for Electronic Excited States Calculations

Chao Yang, Lawrence Berkeley National Laboratory, USA

1:55-2:15 Rational and Polynomial Filtering, Spectrum Slicing, and the EVSL Package

Yousef Saad, University of Minnesota, USA

2:20-2:40 The GW Method for Computing Electronic Excited States of Molecules and Solids

Eric Cances, Ecole des Ponts and Inria, France

Tuesday, February 28

MS128

Stochastic Methods in Computational Science

1:30 PM-3:10 PM

Room:218

In this minisymposium we consider the application of stochastic algorithms in computational science. Stochastic methods are now commonly used for numerical computations in partial differential equations, numerical linear algebra. The methods are often Monte Carlo or quasi- Monte Carlo methods, but include many methods commonly used in the data sciences as well.

Organizer: Michael Mascagni

Florida State University, USA

1:30-1:50 Revisiting Quasi-Standard Error

Hongmei Chi, Florida A & M University, USA

1:55-2:15 Revisit of Block Power Method for Markov Chain Monte Carlo Applications

Yaohang Li, Old Dominion University, USA

2:20-2:40 Analyzing and Improving the Walk-on-Subdomains Algorithm in a Union of Spheres Geometry

Preston Hamlin, Florida State University, USA

2:45-3:05 Stochastic Capacitance Extraction

Chi-Ok Hwang, Gwangju Institute of Science and Technology, Korea

Tuesday, February 28

MS129

Modern Eigenvalue Solvers for Applications in Computational Science and Engineering - Part II of II

1:30 PM-3:10 PM

Room:219

For Part 1 see MS102

A common computational task in many scientific computing applications is the solution of one or more eigenvalues problems. The choice of a solver for a specific problem often depends on the properties and structure of the defining matrices: from large and sparse to relatively small and dense, from single problems to sequences of them. This minisymposium addresses the eigenproblems heterogeneity in connection with the rich variety of modern software packages and implementations which are used to solve them. The ultimate goal is to make computational specialists and computer scientists aware of the current status of research and scientific advancement.

Organizer: Edoardo A. Di Napoli

Jülich Supercomputing Centre, Germany

Organizer: Eric Polizzi

University of Massachusetts, Amherst, USA

Organizer: Yousef Saad

University of Minnesota, USA

1:30-1:50 Recent Advancements and Future Plans for Next-Generation Eigensolvers in Anasazi

Heidi K. Thornquist, Sandia National Laboratories, USA

1:55-2:15 Rational and Polynomial Filtering for Eigenvalue Problems

Yuanzhe Xi and Yousef Saad, University of Minnesota, USA

2:20-2:40 Variance Reduction Through Multigrid Deflation

Andreas Stathopoulos, Eloy Romero, Arjun Gambhir, and Kostas Orginos, College of William & Mary, USA

2:45-3:05 Feast Eigensolver: Practices and Applications

Eric Polizzi, James Kestyn, and Brendan Gavin, University of Massachusetts, Amherst, USA

Tuesday, February 28

MS130

High-Performance Graph Algorithms - Part II of II

1:30 PM-3:10 PM

Room:220

For Part 1 see MS103

Graph algorithms play an important role in the manipulation, distribution and analysis of large data sets arising from both traditional and emerging computational science applications. This minisymposium brings together researchers engaged in developing high-performance parallel graph algorithms with applications to parallel computing, linear system solvers, genomics, neuroscience, and cybersecurity.

Organizer: Karen D. Devine

Sandia National Laboratories, USA

Organizer: Kamesh Madduri

Pennsylvania State University, USA

Organizer: Siva Rajamanickam

Sandia National Laboratories, USA

1:30-1:50 Balanced Multi-Criteria Graph Partitioning

Cedric Chevalier and R*emi Barat*, CEA/DAM, France; Francois Pellegrini, University of Bordeaux, France

1:55-2:15 Multilevel Acyclic Partitioning of Directed Acyclic Graphs for Enhancing Data Locality

Julien Herrmann, Georgia Institute of Technology, USA; Aravind Sukumaran Rajam, Ohio University, USA; Fabrice Rastello, Inria, France; P. (Saday) Sadayappan, Ohio State University, USA; *Umit V. Catalyurek*, Georgia Institute of Technology, USA

2:20-2:40 Partitioning Irregular Graphs at the Trillion-Edge Scale

George M. Slota, Rensselaer Polytechnic Institute, USA; Siva Rajamanickam, Sandia National Laboratories, USA; Kamesh Madduri, Pennsylvania State University, USA; Karen D. Devine, Sandia National Laboratories, USA

2:45-3:05 Sparse Matrix-Matrix Multiplication for Modern Architectures

Mehmet Deveci, Erik G. Boman, and Siva Rajamanickam, Sandia National Laboratories, USA

Tuesday, February 28

MS131

Computational Challenges for Heterogeneous Applications on GPU and KNL - Part II of II

1:30 PM-3:10 PM

Room:Crystal AF - 1st Fl

For Part 1 see MS104

Large-scale computing capabilities are on the horizon, opening up new prospects for Computational Sciences. As hardware moves towards heterogeneous systems, application scientists face many computational challenges in order to use them efficiently. We propose a minisymposium to present the view from leading scientists on how to addresses these issues in selected application areas, such as energy, material design, weather prediction, and CFD-modeling. We will start by exploring multicore/GPU-based architectures and runtime improvements, as a generic way to accelerate applications utilizing linear algebra (especially the eigenvalue problems), and then concentrate on specific applications and their respective challenges from academia and industry.

Organizer: Stanimire Tomov

University of Tennessee, Knoxville, USA

1:30-1:50 GPU Computing in Iterative Solvers for Sparse Linear Systems

Amal Khabou, Aygul Jamal, and Marc Baboulin, University of Paris-Sud, France; Masha Sosonkina, Old Dominion University, USA

1:55-2:15 Exploring Efficient Block-Updates on GPU for Quantum Monte Carlo Simulation

Eduardo F. D'Azevedo, Paul Kent, and Ying Wai, Oak Ridge National Laboratory, USA; Tyler McDaniel, University of North Carolina at Asheville; Kwai L. Wong, University of Tennessee and Oak Ridge National Laboratory, USA

2:20-2:40 Spectral Graph Partitioning and Clustering on the GPU

Maxim Naumov, NVIDIA, USA; Timothy Moon, Stanford University, USA; Alexandre Fender, NVIDIA, USA

2:45-3:05 Performance Evaluation of Time-Space Tiling Strategies for Iterative Stencil Computations on Multi/Many-Core CPU Systems

Takeshi Fukaya and Takeshi Iwashita, Hokkaido University, Japan

Tuesday, February 28

MS132

Advanced Scientific Computing using Julia - Part II of II

1:30 PM-3:10 PM

Room:Crystal CD - 1st Fl

For Part 1 see MS105

This minisymposium showcases recent developments and applications for advanced scientific computing in Julia. Julia is a dynamic high-level language for technical computing, which is increasingly being used for solving complex and large-scale problems. It is developed and maintained by an large and active group of developers from around the world. This minisymposium brings together a wide range of applications of Julia in network analysis, optimization, inverse problems, partial differential equations, and parallel computing.

Organizer: Lars Ruthotto

Emory University, USA

Organizer: Chen Jiahao

Massachusetts Institute of Technology, USA

1:30-1:50 Solving Large-Scale Electromagnetic Inverse Problems

Eldad Haber, University of British Columbia, Canada

1:55-2:15 Lazy Array Computations with Julia

Timothy E. Holy, Washington University in St. Louis, USA

2:20-2:40 Integral Equation Solver for Metamaterial Design

Boaz Blankrot and Clemens Heitzinger, Vienna University of Technology, Austria

2:45-3:05 Networks Analysis Using Julia

Huda Nassar and David F. Gleich, Purdue University, USA

Tuesday, February 28

MS133

Reduced Order Models for Fluids: Achievements and Open Problems - Part II of II

1:30 PM-3:10 PM

Room:301

For Part 1 see MS106

This minisymposium aims at giving a survey of recent developments in the reduced order modeling of fluid flows. Computational modeling, numerical analysis and applications to realistic engineering and geophysical flow problems will be covered in this minisymposium. Both achievements and open problems in the reduced order modeling of fluid flows will be discussed.

Organizer: Traian Iliescu

Virginia Tech, USA

1:30-1:50 Data-Driven, Physics-Constrained Model Reduction of Convection Dominated Flows

Maciej Balajewicz, University of Illinois at Urbana-Champaign, USA; Irina K. Tezaur, Sandia National Laboratories, USA; Earl Dowell, Duke University, USA

1:55-2:15 A Fast Algorithm for Ensemble-Based Reduced Order Simulations of Complex Fluid Flows

Zhu Wang, University of South Carolina, USA

2:20-2:40 An Artificial Neural Network Closure Modeling Framework for Model Order Reduction of Convective Flows

Mansoor Ahmed and *Omer San*, Oklahoma State University, USA

2:45-3:05 A Reduced-Basis Smagorinsky Turbulence Model

Enrique Delgado, Tomas Chacon, and Macarena Gomez, Universidad de Sevilla, Spain

Tuesday, February 28

MS134

Model Order Reduction: Perspectives from Junior Researchers - Part II of II

1:30 PM-3:10 PM

Room:302

For Part 1 see MS107

The increasing demands on computational models, and their ever-growing complexity made model reduction ubiquitous in many areas of computational science and engineering. By exploiting the structure of mathematical models, impressive reductions in state-dimension can be achieved, while retaining important features of the full dimensional model. In this minisymposium, the next generation of young researchers in model reduction presents a breadth of work on new methods, and exciting applications, such as: fluid dynamics, fire simulations, and transport phenomena.

Organizer: Boris Kramer

Massachusetts Institute of Technology, USA

1:30-1:50 Nonlinear Model Reduction via Dynamic Mode Decomposition

Alessandro Alla, Florida State University, USA; Nathan Kutz, University of Washington, USA

1:55-2:15 Iterative Rational Krylov Algorithms for Unstable Dynamical Systems and Optimality Conditions for a Finite-Time Horizon

Klajdi Sinani and Serkan Gugercin, Virginia Tech, USA

2:20-2:40 Using Reduced Order Modeling to Solve an Assortment of Nonlocal Problems

David Witman, Florida State University, USA

2:45-3:05 Model Reduction, Transport Problems and Structure

Benjamin Unger, Technische Universität Berlin, Germany

Tuesday, February 28

MS135

Expanding Computing Science Research through Broader Engagement - Part II of II

1:30 PM-3:10 PM

Room:303

For Part 1 see MS108

The goal of the Broader Engagement program at SIAM CSE17 is to expand the computational science and engineering research community by engaging and supporting students and faculty from nontraditional and underrepresented backgrounds. This minisymposium will describe the Broader Engagement program and will include research presentations from faculty and students participating in the CSE17 Broader Engagement program.

Organizer: Mary Ann E. Leung

Sustainable Horizons Institute, USA

1:30-1:50 Simulation of Shock Wave/ Boundary Layer Interaction Using High Resolution Numerical Scheme

Ovais Khan, Tuskegee University, USA

Additional speakers to be announced.

Tuesday, February 28

MS136

Computational Poromechanics - Part II of II

1:30 PM-3:10 PM

Room:304

For Part 1 see MS109

Despite their central role in many applications, ranging from petroleum to biomedical engineering, the numerical solutions to the PDEs coupling thermal, flow and mechanical processes in porous media are still a challenging task. For instance, the problem of ill-conditioning may arise from large time- and space-scale contrasts, nonlinear material behaviors, heterogeneity, and anisotropy, with an associated significant computational burden. This minisymposium aims at highlighting the current status of research and the recent advances developed to address the main open issues. These may include novel discretization methods, stabilization techniques, original solution algorithms, and inverse coupled modeling.

Organizer: Massimiliano Ferronato

University of Padova, Italy

Organizer: Jinhyun Choo

Stanford University, USA

1:30-1:50 An Oscillation-Free Element-Based Finite Volume Technique for Poroelastic Problems

Herminio Tasinafo Honório, Federal University of Santa Caterina, Brazil; Massimiliano Ferronato and Carlo Janna, University of Padova, Italy; Clovis R. Maliska, Federal University of Santa Caterina, Brazil

1:55-2:15 A Variational Eigen-Deformation Model for Brittle Fractures in Fluid-Infiltrating Porous Media under Non-Isothermal Condition

WaiChing Sun and Kun Wang, Columbia University, USA

continued in next column

2:20-2:40 Coupled Modeling of Flow, Deformation and Heat Transport in Thermo-Hydro-Mechanical Systems

Saro Meguerdijian, University of Southern California, USA

2:45-3:05 Fracture Propagation in Porous Media using Phase Field Approach

Sanghyun Lee, University of Texas at Austin, USA; Andro Mikelić, University of Lyon 1, France; Mary F. Wheeler, University of Texas at Austin, USA; Thomas Wick, Austrian Academy of Sciences, Austria

Tuesday, February 28

MS137

Data-Driven Characterization, Control, and Uncertainty Quantification of Dynamical Systems - Part II of II

1:30 PM-3:10 PM

Room:305

For Part 1 see MS110

Data-driven methods play an increasingly vital role across the physical, engineering and biological sciences. The characterization of dynamical systems from data is an especially vibrant field, with solid theoretical and algorithmic underpinnings and applications to control and uncertainty management in real-world systems. This mini-symposium brings together experts working at the forefront of data-driven methods, which include techniques from machine learning, compressed sensing, dimension reduction, uncertainty quantification, and control. Topics of interest include sensor placement, nonlinear system identification, model selection, and machine learning for control, with diverse applications to the study of flight dynamics, climate systems, epidemiological models, biological regulatory networks, and turbulence.

Organizer: Travis Askham

University of Washington, USA

Organizer: Eurika Kaiser

University of Washington, USA

1:30-1:50 Extraction and Prediction of Coherent Patterns in Incompressible Flows Through Space-Time Koopman Analysis

Dimitrios Giannakis, Courant Institute of Mathematical Sciences, New York University, USA

1:55-2:15 Koopman Operator Framework for Nonlinear System Identification

Amit Surana, Matthew Williams, and Milos Ilak, United Technologies Research Center, USA

2:20-2:40 Data-Driven Adaptive Control of Combustor Instabilities

Ankit Goel, Karthik Duraisamy, and Dennis Bernstein, University of Michigan, Ann Arbor, USA

2:45-3:05 Identifying Anomalous Epidemics with Optimized Models of Sensor Networks

Kyle B. Gustafson and Joshua L. Proctor, Institute for Disease Modeling, USA

continued in next column

Tuesday, February 28

MS138

Automatic Differentiation: Algorithms, Software, and Applications

1:30 PM-3:10 PM

Room:221

Automatic or Algorithmic Differentiation (AD) is a technology for differentiating a function encoded as a computer program by augmenting the program to analytically compute the derivatives efficiently and accurately to machine precision. AD enables the solution of nonlinear optimization problems and differential equations in many applications. Recently new efficient algorithms for computing second and higher order derivatives have been designed; ``structure' in derivatives of functions involving multi-stage computations has been exploited to preserve sparsity; AD tools have been developed for languages such as Python, R, and Julia; and these tools have been applied to emerging application areas such as machine learning, financial optimization, uncertainty quantification, etc. The speakers in this minisymposium will discuss these recent developments.

Organizer: Alex Pothen

Purdue University, USA

1:30-1:50 Structured Automatic Differentiation for Hedging Financial Contracts

Thomas F. Coleman, University of Waterloo, Canada

1:55-2:15 Automatic Differentiation for Machine Learning Applications

Paul D. Hovland, Argonne National Laboratory, USA; Kaitlyn MacIntyre, Northwestern University, USA; Sri Hari Krishn Narayanan, Argonne National Laboratory, USA

2:20-2:40 Binomial Checkpointing for Arbitrary Programs with No User Annotation

Jeffrey Mark Siskind, Purdue University, USA

2:45-3:05 Second and Higher Order Derivatives Using Reverse Mode of Automatic Differentiation

Mu Wang, Purdue University, USA

Tuesday, February 28

MS139

Uncertainty Quantification in Turbulent Flow Simulations - Part II of II

1:30 PM-3:10 PM

Room:222

For Part 1 see MS112

Accurate predictions of turbulent flows are of crucial importance for the design and operation of complex systems such as aircrafts and gas turbine engines. However, it remains challenging to simulate these flows computationally and to estimate system performance with confidence. Prediction uncertainties can emerge from a number of sources, e.g., geometric variability, boundary and initial conditions, and assumptions embedded in engineering models of turbulent motion. This minisymposium aims to bring together researchers working on uncertainty quantification in turbulence modeling and simulations, including (1) input uncertainty, model-from uncertainty, and their coupling, and (2) uncertainties in turbulence modeling approaches of various fidelities.

Organizer: Heng Xiao
Virginia Tech, USA

Organizer: Gianluca Iaccarino
Stanford University, USA

1:30-1:50 A Framework for Epistemic Uncertainty Quantification in Large-Eddy Simulation Closures

Stefan P. Domino, Sandia National Laboratories, USA; Lluis Jofre and *Gianluca Iaccarino*, Stanford University, USA

1:55-2:15 Deep Learning for Turbulence Modeling

Julia Ling, Sandia National Laboratories, USA; Andrew Kurzawski, University of Texas at Austin, USA; Jeremy Templeton, Sandia National Laboratories, USA

2:20-2:40 Estimating and Verifying K-Epsilon Model Coefficients for Jet-in-Crossflow Simulations

Jaideep Ray, Sophia Lefantzi, Julia Ling, Lawrence Dechant, and Srinivasan Arunajatesan, Sandia National Laboratories, USA

2:45-3:05 Bayesian Averaging for Estimating RANS Inadequacy in Large Simulations

Richard Dwght, Technische Universität Delft, Germany

Tuesday, February 28

CP9

Uncertainty Quantification - Part II of IV

1:30 PM-3:10 PM

Room:223

For Part 1 see CP7
For Part 3 see CP11

Chair: To Be Determined

1:30-1:40 Impact of Parametric Uncertainty on Estimation of the Energy Deposition into an Irradiated Brain Tumor

Soren Taverniers and Daniel M. Tartakovsky, University of California, San Diego, USA

1:42-1:52 Mesh Discretization Error and Uncertainty Quantification: A Variational Multiscale Approach

Oriol Colomes and Guglielmo Scovazzi, Duke University, USA

1:54-2:04 Stochastic Model Reduction of Allen-Cahn Phase Field Model with High Dimensional Random Forcing

Mayank Bajpayi, Brown University, USA; Hessam Babaee, Massachusetts Institute of Technology, USA; George E. Karniadakis, Brown University, USA

2:06-2:16 Model Reduction from Partial Observations

Cédric Herzet, Inria Rennes, France; Angélique Drémeau, École nationale supérieure de techniques avancées Bretagne, France; Patrick Héas, Inria, France

2:18-2:28 Transported PDF Approaches for Propagating Parameter Uncertainty: A Reacting Flow Case Study

Hemanth Kolla, Sandia National Laboratories, USA; Xinyu Zhao, University of Connecticut, USA; Habib N. Najm, Sandia National Laboratories, USA

2:30-2:40 A Stochastic Galerkin Method for the Boltzmann Equation with High Dimensional Random Inputs Using Sparse Grids

Ruiwen Shu, University of Wisconsin, USA; Shi Jin, Shanghai Jiao Tong University, China, and the University of Wisconsin-Madison, USA; Jingwei Hu, Purdue University, USA

continued in next column

2:42-2:52 An Incremental Compressive Sampling Approach for Sparser Recovery of Polynomial Chaos Expansions

Hadi Meidani and *Negin Alemazkoor*, University of Illinois at Urbana-Champaign, USA

2:54-3:04 An Information Theoretic Approach to Use High-Fidelity Codes to Calibrate Low-Fidelity Codes

Ralph C. Smith and *Kayla Coleman*, North Carolina State University, USA; Brian Williams, Los Alamos National Laboratory, USA

Tuesday, February 28

CP10

Numerical PDEs - Part II of VI

1:30 PM-3:10 PM

Room:224

For Part 1 see CP8
For Part 3 see CP12

Chair: To Be Determined

1:30-1:40 Polynomial Particular Solutions for Solving Elliptic Partial Differential Equations
Thir R. Dangal and C.S. Chen, University of Southern Mississippi, USA; JI Lin, Hohai University, China

1:42-1:52 Indifference Pricing of a GLWB Option in Variable Annuities
Jungmin Choi, East Carolina University, USA

1:54-2:04 An Efficient Numerical Scheme for Space-Fractional Fitzhugh-Nagumo Model
Olaniyi S. Iyiola and Bruce Wade, University of Wisconsin, Milwaukee, USA; Khaled Furati, King Fahd University of Petroleum and Minerals, Saudi Arabia; Abdul Khaliq, Middle Tennessee State University, USA

2:06-2:16 A Comparison of Adaptive Mesh Refinement Techniques for Poisson's Equation
Shih-Yu Lee, Eugenio Aulisa, and Guoyi Ke, Texas Tech University, USA

2:18-2:28 The Computational Analysis of Problems on Domains with Small Holes
Ana Maria Soane, US Naval Academy, USA; Ivo Babuska, University of Texas at Austin, USA; Manil Suri, University of Maryland, Baltimore County, USA

2:30-2:40 Sub-Linear Time Discrete Sparse Fourier Transform Algorithm
Ruochuan Zhang, Michigan State University, USA

2:42-2:52 Numerical Methods of Rational Form for Solving Partial Differential Equations
Said Algarni, King Fahd University of Petroleum and Minerals, Saudi Arabia

2:54-3:04 Multi-Dimensional Sublinear Spase Fourier Algorithm
Bosu Choi, Michigan State University, USA

Tuesday, February 28

Poster Blitz & Coffee Break

3:10 PM-4:30 PM

Room:Ballroom D - 2nd Fl

PP1

Electronic Posters

4:30 PM-6:30 PM

Room:Galleria

Preconditioning for Incompressible Two-Phase Flow
Niall Bootland, University of Oxford, United Kingdom

Nonlinear Model Reduction in Computational Fluid Dynamics
Kevin T. Carlberg, Sandia National Laboratories, USA

Mixed-Integer PDE-Constrained Optimization
Sven Leyffer, Argonne National Laboratory, USA

JInv - A Flexible Julia Package for Parallel PDE Parameter Estimation
Lars Ruthotto and Samy Wu Fung, Emory University, USA; Eran Treister, Ben Gurion University Negev, Israel; *Eldad Haber*, University of British Columbia, Canada

A Fully-Coupled Discontinuous Galerkin Spectral Element Method for Two-Phase Flow in Petroleum Reservoirs
Ankur Taneja and Jonathan Higdon, University of Illinois at Urbana-Champaign, USA

Exahype - An Exascale Engine for Solving Hyperbolic PDEs: Various Equations and Quick Adaption to the Users' Needs Becoming Open Source
Dominic E. Charrier, Durham University, United Kingdom; Jean-Matthieu Gallard, Technische Universität München, Germany; Sven Köppel, Goethe Universität Frankfurt, Germany; *Vasco Varduhn*, Technische Universität München, Germany; Tobias Weinzierl, Durham University, United Kingdom; Michael Bader, Technische Universität München, Germany

continued in next column

Physically Constrained Kalman Filter
Erin Linebarger and Akil Narayan, University of Utah, USA; Dongbin Xiu, Ohio State University, USA

SpinDoctor: A Simulation Tool for Diffusion MRI
Jing-Rebecca Li, INRIA Saclay, France

Offline-Enhanced Reduced Basis Method Through Adaptive Construction of the Surrogate Parameter Domain
Jiahua Jiang, University of Massachusetts, Dartmouth, USA

Scalable Time-Stepping for PDEs Through Componentwise Approximation of Matrix Functions
James V. Lambers, University of Southern Mississippi, USA

Adaptive Turbulence Simulations with Moving Domains and Multi-Phase Flow, with Applications in Biomechanics and Renewable Energy
Massimiliano Leoni, Johan Hoffman, Johan Jansson, Van Dang Nguyen, and Jeannette Spuhler, KTH Royal Institute of Technology, Sweden

Optimized Least-Squares Rational Filters for Interior Eigenvalue Problems
Jan Winkelmann, RWTH Aachen University, Germany; Edoardo A. Di Napoli, Jülich Supercomputing Centre, Germany

Factorization Based Sparse Solvers and Preconditioners -- Recent Developments for Superlu and Strumpack
Xiaoye Sherry Li and Pieter Ghysels, Lawrence Berkeley National Laboratory, USA; Chris Gorman, University of California, Santa Barbara, USA; Artem Napov, Université Libre de Bruxelles, Belgium; Francois-Henry Rouet, Livermore Software Technology Corporation, USA; Piyush Sao, Georgia Institute of Technology, USA

Scikit-Shape: A Python Package for Shape Optimization and Analysis
Gunay Dogan, National Institute of Standards and Technology, USA

Computing Reduced Order Models Using Randomization
Selin Sariaydin, Eric De Sturler, and Serkan Gugercin, Virginia Tech, USA

Minisymposterium: Solitary Waves and Shock Waves in Periodic and Random Media
David I. Ketcheson, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Tuesday, February 28

PP2

General Posters

4:30 PM-6:30 PM

Room:Galleria

Krylov Subspace Spectral Methods for Navier-Stokes in Cylindrical Geometries

Brianna Bingham and James V. Lambers, University of Southern Mississippi, USA

Galerkin Differences: Very High-Order Accurate and Energy Stable PDE Discretizations

John Jacangelo and Jeffrey W. Banks, Rensselaer Polytechnic Institute, USA

Numerical MOOC: Collaborating in Open Education for CSE

Lorena A. Barba, George Washington University, USA; Ian Hawke, Southampton University, United Kingdom; Bernard Knaepen, Université Libre de Bruxelles, Belgium

A Subspace Pursuit Method to Invert the Refractivity Profile within the Marine Atmospheric Boundary Layer

Marc Aurele T. Gilles, Christopher J. Earls, and David Bindel, Cornell University, USA

Measuring and Modeling Bipartite Graphs with Community Structure

Sinan G. Aksoy, University of California, San Diego, USA; Tamara G. Kolda and Ali Pinar, Sandia National Laboratories, USA

Padé Time-Stepping Methods for Solving Partial Differential Equations

Said Algarni, King Fahd University of Petroleum and Minerals, Saudi Arabia

Nonconforming Immersed Finite Element Spaces For Elliptic Interface Problems

Ruchi Guo and Tao Lin, Virginia Tech, USA

Prestructuring to Eliminate Dense Rows from Sparse Matrices

Jason Howell, College of Charleston, USA

continued in next column

A Weno-Based Method of Lines Transpose Approach for Vlasov Simulations

Yan Jiang, Michigan State University, USA

A Multilevel Low-Rank Preconditioner for Indefinite Linear Systems

Geoffrey Dillon, Yuanzhe Xi, and Yousef Saad, University of Minnesota, USA

Numerical Analysis of Set and Fuzzy Integral Equations and Its Applications

Vira Babenko, Ithaca College, USA

Direct Solution of High-Dimension Sylvester Equations

Tomas Co, Michigan Technological University, USA

A New Goal-Oriented A Posteriori Error Estimation for 2D and 3D Saddle Point Problems in Adaptive Fem hp

Arezou Ghesmati, Texas A&M University, USA; Wolfgang Bangerth, Colorado State University, USA; Bruno Turcksin, Oak Ridge National Laboratory, USA

Iterative Hybrid Methods with Wavelet Denoising

Matthew Brown and Julianne Chung, Virginia Tech, USA

A Generalized Constitutive Relation Error

Mengwu Guo, Tsinghua University, China; Weimin Han, University of Iowa, USA; Hongzhi Zhong, Tsinghua University, China

Computing Particle Trajectories with Full Phase Information in a Magnetic Field by a Multiscale Hybridization Technique Derived from Time-Parallel Computing Methodology

Carl D. Lederman, ERC Inc., USA; David Bilyeu, Air Force Research Laboratory, USA

A Resistive Magneto-Hydrodynamic Numerical Model in the Context of Cell-Averaged Adaptive Multiresolution Methods: Verification Tests

Anna Karina F. Gomes, National Institute for Space Research, Brazil; Margarete Domingues, Instituto Nacional de Pesquisa Espaciais, Brazil; Odim Mendes, Sao Jose dos Campos, SP, Brazil; Kai Schneider, Aix-Marseille Université, France

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A Splitting Discontinuous Galerkin Method for the Coupling of Flow and Geomechanics

Nabil Chaabane, Virginia Tech, USA

MultiMesh: Fem on Arbitrarily Many Intersecting Meshes

August Johansson and Benjamin Kehlet, Simula Research Laboratory, Norway; Mats G. Larson, Umeå University, Sweden; Anders Logg, Chalmers University of Technology, Sweden

Asynchronous Task-Based Parallelization of Algebraic Multigrid

Amani Alonazi and David E. Keyes, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Computational Modeling of Shock Wave Reflections Over a Wedge

Uthman Clark, Tuskegee University, USA

Implicit Unstructured Aerodynamics on Emerging Multi and Many-Core HPC Architectures

Mohammed A. Al Farhan, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Dinesh Kaushik, Qatar Foundation, Qatar; David E. Keyes, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Schur Complement Domain Decomposition for Large Scale Kinetic Transport Problems

Charles K. Garrett, Los Alamos National Laboratory, USA; Kevin Procopio, University of Pennsylvania, USA

New Clustering Algorithms to Identify Nonlinear Behavior During a Car Crash Simulation

Dennis Grunert and Joerg Fehr, Universität Stuttgart, Germany

Dislocation Dynamics Simulations of Void and Precipitate Strengthening

Joshua C. Crone, James J. Ramsey, and Jaroslaw Knap, US Army Research Laboratory, USA

Validation of Large Fluid Dynamic Simulations of Complex Geometries with 3D Printing

John Gounley, Duke University, USA; Rafeed Chaudhury, Priya Nair, Girish Pathangey, and Kevin Winarta, Arizona State University, USA; Justin Ryan, Phoenix Children's Hospital, USA; Erik W. Draeger, Lawrence Livermore National Laboratory, USA; David Frakes, Arizona State University, USA; Amanda Randles, Duke University, USA

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Acceleration of a Multiscale Model of An Energetic Material Through Speculative Computation

Kenneth Leiter and Jaroslaw Knap, US Army Research Laboratory, USA; Brian Barnes, U.S. Army Research Laboratory, USA; Claire Eisner and Richard Becker, US Army Research Laboratory, USA

Project Research Model Canvas An Auxiliary Tool to Create and Manage Research Projects

Hiago A. Silva, *Alexandre Cardoso*, and Edgard Lamounier, Federal University of Uberlandia, Brazil

Setting Tunable Solver Parameters with Performance Models

Hormozd Gahvari, Lawrence Livermore National Laboratory, USA; William D. Gropp, University of Illinois at Urbana-Champaign, USA; Kirk E. Jordan, IBM T.J. Watson Research Center, USA; Jacob B. Schroder, Martin Schulz, and Ulrike M. Yang, Lawrence Livermore National Laboratory, USA

Nonnegative Sparse Tensor Decomposition on Distributed Memory Systems

Jiajia Li, Georgia Institute of Technology, USA; Jee Choi and Xing Liu, IBM Research, USA; Richard Vuduc, Georgia Institute of Technology, USA

Methodology for Optimized Generation of Virtual Environments Based on Hydroelectric Power Plants

Ígor A. Andrade Moraes, Alexandre Cardoso, Edgard Afonso Lamounier Jr, and Milton Miranda Neto, Federal University of Uberlandia, Brazil

A Strategy to Improve 3D Arrangement Modeling on Virtual Electrical Substations

Camilo Lellis Barreto Junior, *Alexandre Cardoso*, Edgard Lamounier, and Nicholas Duboc, Federal University of Uberlandia, Brazil; Paulo Prado, Energy Company of Minas Gerais, Brazil

Fast and Efficient Hyperbolic Embeddings for Large Graphs

Kenny Chowdhary, Sandia National Laboratories, USA

continued in next column

A Virtual Reality Based Approach to Improve Human Performance and to Minimize Safety Risks When Operating Power Electric Systems

Alexandre C. Silva, *Alexandre Cardoso*, and Edgard Lamounier, Federal University of Uberlandia, Brazil; Paulo Prado, Energy Company of Minas Gerais, Brazil; Milton Miranda, Gerson Lima, Camilo Barreto, and Nicholas Duboc, Federal University of Uberlandia, Brazil

Stochastic Simulation of Multilevel Monte Carlo on Multi-GPU Systems

Jj Lay, Middle Tennessee State University, USA

Condition Assessment and Prognosis Using Fluid-Structure Interaction Model Updating Within a Stochastic Inversion Framework

Justyna Kosianka and Christopher Earls, Cornell University, USA

Second-Order Langevin Markov Chain Monte Carlo

Thomas A. Catanach and James Beck, California Institute of Technology, USA

Bayesian Optimization with a Finite Budget: An Approximate Dynamic Programming Approach

Remi Lam and Karen E. Willcox, Massachusetts Institute of Technology, USA; David Wolpert, Santa Fe Institute, USA

Computational Advances by Variational Formulation for Breast Cancer Detection Through Electrical Impedance Tomography

Vladislav Bukshtynov and Ugur G. Abdulla, Florida Institute of Technology, USA

Electrical Impedance Tomography for Damage Detection in Concrete

Sanwar Ahmad and Tao Ruan, Clemson University, USA; Thilo Strauss, University of Washington, USA

A Numerical Method for High Energy X-Ray Source Shape Reconstruction

Jesse Adams, University of Arizona, USA

Locally Adaptive Discriminant Analysis

Margaret C. Hock, University of Alabama, Huntsville, USA; Marylesa Howard and Tim Meehan, National Security Technologies, LLC, USA

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A Simplified Human Birth Model: Translation of a Rigid Cylinder Through a Passive Elastic Tube

Roseanna Gossmann, Tulane University, USA; Alexa Baumer, George Washington University, USA; Lisa J. Fauci, Tulane University, USA; Megan C. Leftwich, George Washington University, USA

Finite Volume Methods for Visco-Plastic Flow and Dispersive Waves

Jihwan Kim, University of Oslo, Norway

Resolution Analysis of Pod-Based Imaging Using Tikhonov Regularized Geophysical Inversion

Shyla R. Kupis, Stephen Moysey, and Taufiquar Khan, Clemson University, USA

Identification of Gene Regulatory Models Using Data-Driven Reduction of the Chemical Master Equation

Zachary Fox, Colorado State University, USA; Ania-Ariadna Baetica, California Institute of Technology, USA; Huy D. Vo, University of Alabama, USA; Brian Munsky, Colorado State University, USA

Pricing and Hedging in a Stochastic Volatility Model with Finite Element Method

Jungmin Choi, East Carolina University, USA

Simulation of Rarefied Gases Using Hyperbolic Moment Models

Julian Koellermeier and Manuel Torrilhon, RWTH Aachen University, Germany

Diffusion Mri in the Aplysia Neuronal Network: Experiments & Numerical Simulations

Jing-Rebecca Li, INRIA Saclay, France; Khieu Van Nguyen and Luisa Ciobanu, CEA Saclay, France; Denis Le Bihan, CEA-Neurospin, France

Explicit Continuous Finite Element Methods on Triangles

Jay M. Appleton and Brian Helenbrook, Clarkson University, USA

Melting-Refreezing Cycles of Sea Water Ice – An Enthalpy-Based Fixed Grid Approach

Julia Kowalski, Marco Schoos, and Alexander Gary Zimmermann, RWTH Aachen University, Germany

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Tuesday, February 28

PP2

General Posters

4:30 PM-6:30 PM

continued

Convergence Study for Stochastic Inversion Framework to Monitor Evolving Surface Ship Mass Properties During Arctic Operations

Yolanda C. Lin and Christopher Earls, Cornell University, USA

The Stability Region for Feedback Control of the Wake Behind Twin Oscillating Cylinders

Jeff Borggaard, Serkan Gugercin and Lizette Zietsman, Virginia Tech, USA

Shape-Memory Polymers: A 3D Phenomenological Constitutive Model for Engineering Applications

Elisa Boatti, Harvard University, USA; Giulia Scalet and Ferdinando Auricchio, University of Pavia, Italy

Simulation of Cerebrospinal Fluid Flow Using Finite Pointset Method

Emmanuel O. Akinlabi, African Institute for Mathematical Sciences, Nigeria

Alternative Algebraic Structures for Modelling and Computation

Jean-Baptiste Latre, CERFACS, France; Philippe Ricoux, TOTAL SA, France; Fraçoise Chatelin, CERFACS, France

A Two Phase Approach for Modeling Sedimentation of Pigments in Liquid Coating Formulations

Emmanuel O. Asante-Asamani, Drake University, USA; Bruce Wade and Lei Wang, University of Wisconsin, Milwaukee, USA

Validated Computation of Topological Entropy in Hybrid Dynamical Systems

Shane D. Kepley and William D. Kalies, Florida Atlantic University, USA

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A Real-Time Automatic Characterization of Fractures in Enhanced Geothermal Systems Using Machine-Learning Technique

Youzuo Lin, Los Alamos National Laboratory, USA; Jayaraman Thiagarajan, Lawrence Livermore National Laboratory, USA; George Guthrie, Los Alamos National Laboratory, USA

Compressed Sensing with Corrupted Measurements and Its Application to Uncertainty Quantification

Casie Bao and Ben Adcock, Simon Fraser University, Canada

Multilevel Stochastic Collocation in Linear Gyrokinetics

Ionut-Gabriel Farcas and Hans-Joachim Bungartz, Technische Universität München, Germany; Tobias Goerler, Max Planck Institute for Plasma Physics, Germany; Denis Jarema and Tobias Neckel, Technische Universität München, Germany

Efficient Computation of Sobol' Indices for Stochastic Models

Joseph L. Hart, Pierre Gremaud, and Alen Alexanderian, North Carolina State University, USA

Tuesday, February 28

PP3

General Posters

4:30 PM-6:30 PM

Room:Galleria

Analytical Stacked Gaussian Process Model

Kareem Abdelfatah, Junshu Bao, and Gabriel Terejanu, University of South Carolina, USA

Uncertainty Quantification in Multi-Scale Materials Modeling

Manuel Aldegunde and Nicholas Zabaras, University of Notre Dame, USA

Near-Optimal Sampling Approach for Estimating Sparse Polynomial Chaos Expansions

Negin Alemazkoor and Hadi Meidani, University of Illinois at Urbana-Champaign, USA

Selective Time Step Adaptivity for Non-Linear Reactive Transport Problems

Yerlan Amanbek, Gurpreet Singh, and Mary F. Wheeler, University of Texas at Austin, USA

Upwind Dissipation for Stability on Composite Grids

Jordan B. Angel, Rensselaer Polytechnic Institute, USA

Fully Bayesian Deep Gaussian Processes for Uncertainty Quantification

Steven Atkinson and Nicholas Zabaras, University of Notre Dame, USA

Polynomial Filtering for Large, Sparse SVD Computations

Anthony P. Austin, Argonne National Laboratory, USA; Jared Aurentz, Instituto de Ciencias Matemáticas, Spain; Vasileios Kalantzis, University of Minnesota, USA

The "Porous Media Initiative" (OPM) Software

Markus Blatt, HPC-Simulation-Software & Services, Germany; Atgeirr Rasmussen, SINTEF ICT, Norway

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The Reduced Collocation Method for Nonlinear Steady-State PDEs
Chris Bresten, University of Massachusetts, Dartmouth, USA; Yanlai Chen, Brown University, USA

Neutrino Radiation Hydrodynamics in Genasis
Reuben Budiardja, University of Tennessee, USA; Christian Cardall and Eirik Endeve, Oak Ridge National Laboratory, USA; Daniel Murphy, University of Tennessee, USA

Numerical Simulations for Fluid-Structure Interaction Modeling of Artery Aneurysms
Sara Calandrini and Eugenio Aulisa, Texas Tech University, USA

Modeling Multiphase Buoyancy Driven Plume Migration During Geologic Co2 Injection
Kyle Campbell, Christopher Paolini, and Jose Castillo, San Diego State University, USA

A Parallel Particle Tracking Algorithm for Finite Element Applications
Giacomo Capodaglio and Eugenio Aulisa, Texas Tech University, USA

Why Is the Ensemble Adjoint Approach to Sensitivity Analysis Not Practical in Chaotic Systems?
Nisha Chandramoorthy and Qiqi Wang, Massachusetts Institute of Technology, USA

A Novel Speech-Based Diagnostic Test for Parkinson's Disease Integrating Machine Learning with Application Development for Cloud Deployment
Pooja Chandrashekar, Harvard University, USA

Protein NMR Reference Correction: A Statistical Approach for an Old Problem
XI Chen, University of Kentucky, USA; Andrey Smelter, University of Louisville, USA; Hunter Moseley, University of Kentucky, USA

Numerical Solutions of Basic Boundary-Contact Problems of Tumor-Brain Interface Tissues
Manana Chumburidze and David Lekveishvili, Akaki Tsereteli State University, Georgia

Horsetail Matching: A Flexible Approach to Optimization Under Probabilistic and Interval Uncertainties
Laurence W. Cook, Massachusetts Institute of Technology, USA; Jerome P. Jarrett, University of Cambridge, United Kingdom; Karen E. Willcox, Massachusetts Institute of Technology, USA

Accelerating Multiplication of Small Or Skinny Matrices with Intel® Math Kernel Library Packed GEMM Routines
Timothy B. Costa, Murat E. Guney, Sarah Knepper, and Shane Story, Intel Corporation, USA

A Mathematical Model of Hemostasis
Nicholas Danes and Karin Leiderman, Colorado School of Mines, USA

An IDS Study of Flow over A Leading Edge
David Dodoo-Amoo, Julio C. Mendez, and Frederick Ferguson, North Carolina A&T State University, USA

Higher Order Asymptotic for Burgers Equation
Satyanarayana Engu, National Institute of Technology Karnataka , Surathkal, India

A Bi-Fidelity, Low-Rank Approximation Technique for Uncertainty Quantification
Hillary Fairbanks, Jerrad Hampton, and Alireza Doostan, University of Colorado Boulder, USA; Akil Narayan, University of Utah, USA

Boundary Integral and Image-Moment Hybrid Method for Simulations of Solvated Proteins
Zecheng Gan, University of Michigan, USA; Weihua Geng, Southern Methodist University, USA; Robert Krasny, University of Michigan, Ann Arbor, USA

Asynchronous Optimized Schwarz Method for Poisson Equation in Rectangular Domains
Jose C. Garay and Daniel B. Szyld, Temple University, USA

Mathematical Analysis of Sludge Disintegration
Rubayyi Alqahtani, Imam University, Saudi Arabia

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Tuesday, February 28

PP101

Minisymposterium: Advanced Numerical Methods for Multiscale Plasma Physics

4:30 PM-6:30 PM

Room:Galleria

Organizers:
Gian Luca Delzanno, Los Alamos National Laboratory, USA

Gianmarco Manzini, Los Alamos National Laboratory, USA

Minisymposterium: Semi-Lagrangian Solution of the Gyrokinetic Vlasov Equation: Field-Aligned Interpolation And Splitting in Complex Geometry
Edoardo Zoni, Technische Universität München, Germany; *Yaman Güçlü,* Max-Planck-Institut für Plasmaphysik, Germany; Michel Mehrenberger, University of Strasbourg, France; Eric Sonnendrücker, Max-Planck-Institut für Plasmaphysik and Technische Universität München, Germany

Minisymposterium: Spectral Based-Discontinuous Galerkin Discretizations of the Vlasov-Poisson System
Gianmarco Manzini and Gian Luca Delzanno, Los Alamos National Laboratory, USA

Minisymposterium: New Hybrid Method for the Vlasov-Maxwell System: Coupling of Spectral and Pic Methods
Oleksandr Koshkarov, University of Saskatchewan, Canada; Gian Luca Delzanno and Gianmarco Manzini, Los Alamos National Laboratory, USA; Vadim Roytershteyn, Space Science Institute, USA

Minisymposterium: Large-Scale Implicit Particle-in-Cell Simulations of Magnetospheres with iPIC3D
Stefano Markidis, Ivy Bo Peng, and Erwin Laure, KTH Royal Institute of Technology, Sweden; Elin Eriksson, Andreas Johlander, Yuri Khotyaintsev, and Andris Vaivads, Uppsala University, Sweden; Gian Luca Delzanno, Los Alamos National Laboratory, USA

Minisymposterium: Computational Ideal Magnetohydrodynamics with FV-FEEC Discretizations
Cecilia Pagliantini, Unaffiliated; Ralf Hiptmair and Siddhartha Mishra, ETH Zürich, Switzerland

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Tuesday, February 28

PP101

Minisymposterium: Advanced Numerical Methods for Multiscale Plasma Physics

4:30 PM-6:30 PM

continued

Minisymposterium: Eulerian Algorithms for the Discretization of Plasma Kinetic Equations

James Juno and Jason TenBarge, University of Maryland, USA; Ammar Hakim, Princeton Plasma Physics Laboratory, USA; William Dorland, University of Maryland, USA

Minisymposterium:Kinetic Simulations of Astrophysical Plasma Turbulence

Vadim Roytershteyn, Space Science Institute, USA

Tuesday, February 28

PP102

Minisymposterium: Advances in Quadrilateral and Hexahedral Finite Elements

4:30 PM-6:30 PM

Room:Galleria

Organizer:

Andrew Gillette, University of Arizona, USA

Minisymposterium: Two Families of H(div) Mixed Finite Elements of Minimal Dimension on Quadrilaterals

Todd Arbogast, University of Texas at Austin, USA; Maicon R. Correa, University of Campinas, Brazil; Zhen Tao, University of Texas at Austin, USA

Minisymposterium: Bernstein-B\'ezier Basis for H(div) and H(curl) Finite Elements on Hypercubes

Guosheng Fu and Mark Ainsworth, Brown University, USA

Minisymposterium: Trimmed Serendipity Finite Elements

Tyler Kloefkorn and Andrew Gillitte, University of Arizona, USA

Minisymposterium: A Progress Report on Construction of Smooth Generalized Barycentric Coordinates

Ming-Jun Lai, University of Georgia, USA

Minisymposterium: Divergence-Free Stokes Elements on Quadrilateral Meshes

Michael J. Neilan and Duygu Sap, University of Pittsburgh, USA

Minisymposterium: Approximation on Quadrilateral and Hexahedral Meshes

Douglas N. Arnold, University of Minnesota, USA

Tuesday, February 28

PP103

Minisymposterium: Clawpack and GeoClaw - Software Developments and Applications

4:30 PM-6:30 PM

Room:Galleria

Organizer:

Randall LeVeque, University of Washington, USA

Minisymposterium: ForestClaw : Parallel Library for Solving Pdes on Mapped Multiblock Quadtree Grids

Donna Calhoun, Boise State University, USA; Carsten Burstedde, Universität Bonn, Germany

Minisymposterium: Simulations of Asteroid-Generated Tsunamis Using GeoClaw

Randall LeVeque, University of Washington, USA; Marsha Berger, Courant Institute of Mathematical Sciences, New York University, USA

Minisymposterium: Embedding Protective Mechanisms in Coastal Flooding Simulations

Kyle T. Mandli and Jiao Li, Columbia University, USA

Minisymposterium: A Combined Model for Sediment Transport In Coastal Hazard Events (GeoClaw-Striche): Theoretical Formulation and Validation

Hui Tang and Robert Weiss, Virginia Tech, USA

Minisymposterium: Seismic Modeling to Improve Tsunami Prediction in Geoclaw

Chris Vogl and Randy LeVeque, University of Washington, USA

Minisymposterium: Clawpack and GeoClaw - Software Developments and Applications - Numerical Prediction of Water Level and Hydrodynamic Loads in Coastal Communities During a 500-Year Csz Tsunami

Xinsheng Qin, University of Washington, Seattle, USA; Michael Motley, Randall LeVeque, and Frank Gonzalez, University of Washington, USA

Tuesday, February 28

PP104

Minisymposterium: Mesoscale Computational Approaches for Heterogeneous Materials

4:30 PM-6:30 PM

Room:Galleria

Organizer:

Paul Atzberger, University of California, Santa Barbara, USA

Minisymposterium: Efficiently Exploring the Conformational Space of Proteins Using the Concurrent Adaptive Sampling Algorithm

Surl-Hee Ahn, Stanford University, USA; Jay Grate, Pacific Northwest National Laboratory, USA; Eric F. Darve, Stanford University, USA

Minisymposterium: Mesh Refinement and Model Reduction: Two Sides of the Same Problem

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

Minisymposterium: Mesoscopic Modeling, Concurrent Coupling and Multiscale Framework

Zhen Li, Brown University, USA; Xin Bian, Technische Universität München, Germany; Yu-Hang Tang and George E. Karniadakis, Brown University, USA

Minisymposterium: Numerical Exterior Calculus Methods for Fluctuating Hydrodynamics Within Curved Fluid Interfaces

Paul J. Atzberger and *Ben J. Gross*, University of California, Santa Barbara, USA

Minisymposterium: A Coupling Strategy for Nonlocal and Local Models

Marta D'Elia, *Pavel Bochev*, Mauro Perego, and David Littlewood, Sandia National Laboratories, USA

Minisymposterium: Computing the Non-Markovian Coarse-Grained Interactions Derived from the Mori-Zwanzig Formalism in Molecular Systems: Application to Polymer Melts

Hee Sun Lee, Stanford University, USA; Zhen Li, Brown University, USA; Eric F. Darve, Stanford University, USA; George E. Karniadakis, Brown University, USA

Minisymposterium: Particle Methods for the Mesoscale

Nathaniel Trask, Sandia National Laboratories, USA; Martin Maxey, Brown University, USA; Alexandre M. Tartakovsky and Wenxiao Pan, Pacific Northwest National Laboratory, USA; George E. Karniadakis, Brown University, USA

Minisymposterium: Effect of Uncertainties in Radii and Atomic Charges on the Solvation Calculations

Xiu Yang, Huan Lei, Peiyuan Gao, and Dennis Thomas, Pacific Northwest National Laboratory, USA; David Mobley, University of California, Irvine, USA; Nathan Baker, Pacific Northwest National Laboratory, USA

Minisymposterium: Fast Hierarchical Solvers for Dense Linear Systems

Hadi Pouransari, Pieter Coulier, and Eric F. Darve, Stanford University, USA

Minisymposterium: A Multifidelity Approach to Effectively Compute Steady-State Flow Of Ionic Solutions

James Cheung, Florida State University, USA; Amalie Frischknecht, *Mauro Perego*, and Pavel Bochev, Sandia National Laboratories, USA

Minisymposterium: Quantifying Quasi-Equilibrium and Non-Equilibrium Properties of Biomolecule System

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

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Tuesday, February 28

PP105

Minisymposterium: Parallel Computing for Models using Partial Differential Equations

4:30 PM-6:30 PM

Room:Galleria

Organizer:

Matthias K. Gobbert, University of Maryland, Baltimore County, USA

Minisymposterium: Performance Comparisons of Application Codes on Modern Computer Architectures

Ishmail Jabbie, University of Maryland, Baltimore County, USA; George Owen, Louisiana State University, USA; Benjamin Whiteley, University of Maryland, Eastern Shore, USA; Jonathan Graf, Xuan Huang, *Matthias K. Gobbert*, and Samuel Khuvis, University of Maryland, Baltimore County, USA

Minisymposterium: Performance Analysis and Numerical Method Tuning for a System of Non-Linear Time-Dependent Advection-Diffusion-Reaction Equations

Jonathan Graf and Matthias K. Gobbert, University of Maryland, Baltimore County, USA

Minisymposterium: Coupling the Electrical Excitation and Calcium Signaling in a Heart Cell

Uchenna Osia, University of Maryland, Baltimore County, USA; Kallista Angeloff, University of Washington, USA; Carlos Barajas, Olivet College, USA; Alexander Middleton, Winthrop University, USA; Jonathan Graf and Matthias K. Gobbert, University of Maryland, Baltimore County, USA; Zana Coulibaly, University of California, Davis, USA

Minisymposterium: Performance Comparison of Intel Xeon Phi Knights Landing

George Owen, Louisiana State University, USA; Ishmail Jabbie, University of Maryland, Baltimore County, USA; Benjamin Whiteley, University of Maryland, Eastern Shore, USA; Jonathan Graf, Matthias K. Gobbert, and Samuel Khuvis, University of Maryland, Baltimore County, USA

Tuesday, February 28

PP106

Minisymposterium: Theory, Numerical Methods and Applications for Sturm Liouville

4:30 PM-6:30 PM

Room:Galleria

Organizer:
Charles T. Fulton, Florida Institute of Technology, USA

Minisymposterium: Eigenvalue Computation for 4th Order Sturm Liouville Equations: Magnus Methods
Ahmad A. Alalyani, Florida Institute of Technology, USA

Minisymposterium: A Sturm Liouville Problem for Relativistic Electrons Inside Thunderstorms
Eric S. Cramer, University of Alabama, Huntsville, USA

SISC Dinner Meeting (by invitation only)

7:00 PM-10:00 PM

Room:Crystal BE

Wednesday, March 1

CSE Book Series Breakfast Meeting (by invitation only)

7:00 AM-8:00 AM

Room:Crystal Boardroom - 1st Fl

Registration

7:30 AM-5:00 PM

Room:Foyer - 1st Fl

Announcements

8:10 AM-8:15 AM

Room:Grand Ballroom - 2nd Fl

Wednesday, March 1

IP5

Multiscale Modelling: Powerful Tool or Too Many Promises

8:15 AM-9:00 AM

Room:Grand Ballroom - 2nd Fl

Chair: Wil Schilders, Technische Universiteit Eindhoven, The Netherlands

Multiscale modelling aims to provide systematic linking of different time and length scales in order to enable simulations at different levels of spatial and/or temporal resolutions. No single unique method exists – or is even foreseeable – and hence the choice of the most appropriate method or mapping depends on the properties of interest. The roots of multiscale simulations go back to the 1960's and 1970's, but the last decade has been brought them in the mainstream of method development and as a viable approach to model complex systems. It has been applied to viral capsids, fluid flow, crystal growth, proteins, colloids, and polymers to mention a few examples. Current techniques range from pragmatic, such as using solubilities for force field mapping to algorithmic, using equilibrium particle data for solving an inverse problem (using methods such as Inverse Boltzmann, force matching and Inverse Monte Carlo), particle-continuum coupling and using Langevin and Fokker-Planck equations and mapping procedure. Procedures such as GENERIC also extend the multiscale approach to irreversible processes. In this talk, I will discuss multiscale methods from the perspective of soft materials based on our own work, provide perspectives for future development and problems involving multiscaling.

Mikko Karttunen
Eindhoven University of Technology, Netherlands

Intermission

9:00 AM-9:10 AM

Wednesday, March 1

MT5

Julia: Technical Computing Made Fast, Flexible, and Easy

9:10 AM-10:50 AM

Room:Ballroom C - 2nd Fl

Chair: Alan Edelman, Massachusetts Institute of Technology and Julia Computing, USA

Julia is a high-level, high-performance dynamic programming language for technical computing, with syntax that is familiar to users of other technical computing environments, yet the under-the-hood architecture is very different from other environments. Julia gains its speed, flexibility, and ease of use in part through multiple-dispatch technology. We all like fast algorithms. They tend to start off on whiteboards. We then implement them with an idea in mind. Perhaps we will work on a small problem, on a laptop, in double precision, for example. Your supervisor wants it done yesterday, and that is all you see. Then it is successful, and you want it to work on larger problems, on GPUs, in distributed memory, and in quad precision. You want to go into productions and have the solution work well beyond the original prototype. Julia is of note for its solution to the two language problem, sometimes known as Ousterhout's dichotomy. In this introductory minitutorial, we will teach Julia, how to use it, its design, and explain why it is becoming the language of choice for Finance, The Internet of Things, Big data, Machine learning, and so much more in Computational Science.

Speakers:

Alan Edelman
Massachusetts Institute of Technology and Julia Computing, USA

David P. Sanders
National University of Mexico, Mexico

Andreas Noack
Massachusetts Institute of Technology, USA

Jarrett Revels
Massachusetts Institute of Technology, USA

Wednesday, March 1

MS140

Probabilistic Machine Learning Tools in Computational Science and Engineering - Part I of II

9:10 AM-10:50 AM

Room:Grand Ballroom - 2nd Fl

For Part 2 see MS168

The never-ending increase of computing power, in combination with the pressing need for robust tools to distill information from data with quantified uncertainty, has put probabilistic machine learning at the epicenter of disruptive developments across many scientific disciplines. Mathematics and engineering in particular, are currently undergoing a steady transition towards which probabilistic data-driven methods come to be viewed as the natural tools to use in computing under uncertainty. This minisymposium invites contributions that showcase the potential of machine learning tools in applied science, including topics in design, uncertainty quantification, inverse problems, and control.

Organizer: Paris Perdikaris
Massachusetts Institute of Technology, USA

Organizer: Ilias Bilionis
Purdue University, USA

9:10-9:30 The Parallel Knowledge Gradient Method for Batch Bayesian Optimization
Jian Wu, Cornell University, USA

9:35-9:55 Data and the Computational Modeling of Complex/Multiscale Systems
Ioannis Kevrekidis, Princeton University, USA

10:00-10:20 Probabilistic, Coarse-Grained Models for PDEs with Random Coefficients
Constantin Grigo and Phaedon S. Koutsourelakis, Technische Universität München, Germany

10:25-10:45 Deep Gaussian Processes for Uncertainty Quantification
Nicholas Zabaras and Steven Atkinson, University of Notre Dame, USA

Wednesday, March 1

MS141

Computational Electrodynamics for Materials and Complex Media

9:10 AM-10:50 AM

Room:Ballroom D - 2nd Fl

This minisymposium seeks to address recent advances in the modeling and numerical simulation of light-matter interaction. High accuracy, stable methods are of particular interest in the design and frequency response optimization of optical devices. Topics of interest include high-order numerical methods in the time domain and at complex material interfaces, simulation of surface plasmonic effects in metamaterials, fluid descriptions of electrons in metals and plasmas, and dispersive Schrodinger descriptions of photonic devices.

Organizer: Michael Jenkinson
Rensselaer Polytechnic Institute, USA

9:10-9:30 Pulse Slowdown in Two-Dimensional Active Media
Gregor Kovacic, Rensselaer Polytechnic Institute, USA

9:35-9:55 High-Order Finite-Difference Time-Domain Simulation of Electromagnetic Waves with Emphasis on Interfaces Between Dispersive Optical Media
Michael Jenkinson, Rensselaer Polytechnic Institute, USA

10:00-10:20 Title Not Available at Time of Publication
Vrushali A. Bokil, Oregon State University, USA

10:25-10:45 Title Not Available at Time of Publication
Jinjie Liu, Delaware State University, USA

Wednesday, March 1

MS142

Advances in Numerical Methods and Algorithms for Radiation Transport - Part I of II

9:10 AM-10:50 AM

Room:202

For Part 2 see MS169

Radiative transfer and radiation transport modelling play an important role in a variety of physical, chemical, and engineering applications. Due to the equations' large phase space, numerical simulations of transport phenomena are still a formidable challenge in terms of discretization techniques, iterative solution processes, and associated algorithms. This minisymposium intends to bring together researchers from applied mathematics, computational science, physics, and engineering communities to discuss recent advances in computational transport methods (PN, discrete ordinates, Monte-Carlo, iterative approaches) and algorithms for large-scale transport simulations.

Organizer: Jean C. Ragusa

Texas A&M University, USA

Organizer: José Pablo Lucero Lorca

Universität Heidelberg, Germany

9:10-9:30 GPU Algorithms for Monte Carlo Particle Transport

Steven Hamilton, Thomas Evans, and Stuart Slattery, Oak Ridge National Laboratory, USA

9:35-9:55 A Fully Synchronous Domain Decomposed Transport Algorithm with Splitting

Tara Pandya and Thomas Evans, Oak Ridge National Laboratory, USA; J. Austin Ellis, North Carolina State University, USA; Seth Johnson, Oak Ridge National Laboratory, USA

10:00-10:20 Adaptive Time Step Selection in Radiative Transfer Calculations

Peter G. Maginot, Lawrence Berkeley National Laboratory, USA

10:25-10:45 A Fast Iterative Method for Non-Linear LTE Radiative Transfer Problems

José Pablo Lucero Lorca and Guido Kanschat, Universität Heidelberg, Germany

Wednesday, March 1

MS143

Sensitivity Analysis and Uncertainty Quantification of Large-Scale Chaotic Flow Simulations - Part I of II

9:10 AM-10:50 AM

Room:203

For Part 2 see MS170

Chaotic dynamics appears in many scientific and engineering applications. Turbulent fluid flows is a prominent example that attracted significant interest both in science and engineering. Sensitivity analysis of these turbulent and chaotic flow simulations help us understand how the quantities of interest respond to geometry, environmental conditions, simulation parameters, and numerical discretization. Uncertainty quantification of these simulations help us assess the accuracy of quantities predicted by these simulations. Sensitivity analysis and uncertainty quantification has special challenges in chaotic simulations, including turbulent flow simulations, because they are exponentially sensitive to initial condition, and exhibit apparently stochastic behavior. In this minisymposium, the speakers illustrate these challenges and progress in new mathematical techniques developed to overcoming these challenges.

Organizer: Qiqi Wang

Massachusetts Institute of Technology, USA

Organizer: Nicolas R. Gauger

Technische Universität Kaiserslautern, Germany

9:10-9:30 Adjoint-Based Sensitivity Analysis of Unsteady and Chaotic Flows in Fun3d

Eric Nielsen, NASA Langley Research Center, USA

continued in next column

9:35-9:55 Adjoint and Tangent Methods in a Higher-Order Space-Time Discontinuous-Galerkin Solver for Turbulent Flows

Laslo Diosady, Scott Murman, Patrick J. Blonigan, and Anirban Garai, NASA Ames Research Center, USA

10:00-10:20 Adjoint Sensitivity Analysis for Scale-Resolving Turbulent Flow Solvers

Patrick J. Blonigan, Laslo Diosady, Anirban Garai, and Scott Murman, NASA Ames Research Center, USA

10:25-10:45 Sensitivity of Wakes Via Global Stability Analysis, Covariant Lypanuov Vectors and Shadowing Method

Luca Magri, Stanford University, USA; Georgios Rigas, California Institute of Technology, USA; Lucas Esclapez, Stanford University, USA; Qiqi Wang, Massachusetts Institute of Technology, USA

Wednesday, March 1

MS144

Software Productivity and Sustainability for CSE and Data Science - Part I of II

9:10 AM-10:50 AM

Room:204

For Part 2 see MS171

Software is the key crosscutting technology that connects advances in mathematics, computer science, and domain-specific science and engineering to achieve robust simulations and analysis for predictive science, engineering, and other research fields. While software is becoming more complex due to multiphysics and multiscale modeling, the coupling of data analytics, and disruptive changes in computer hardware (due to increases in typical system scale and heterogeneity, including GPUs and additional alternative architectures), software itself has not traditionally received focused attention in the CSE community or been rewarded by that community. The speakers in this minisymposium will discuss work that addresses growing technical and social challenges in software productivity, quality, and sustainability, and thereby is helping software to fulfill its critical role as a cornerstone of long-term CSE collaboration.

Organizer: David E. Bernholdt
Oak Ridge National Laboratory, USA

Organizer: Michael Heroux
Sandia National Laboratories, USA

Organizer: Daniel S. Katz
University of Illinois at Urbana-Champaign, USA

Organizer: Lois Curfman McInnes
Argonne National Laboratory, USA

9:10-9:30 CSE Software Ecosystems: Critical Instruments for Scientific Discovery

Lois Curfman McInnes, Argonne National Laboratory, USA; Michael Heroux, Sandia National Laboratories, USA; David Moulton, Los Alamos National Laboratory, USA; David E. Bernholdt, Oak Ridge National Laboratory, USA; Xiaoye Sherry Li, Lawrence Berkeley National Laboratory, USA; Timothy D. Scheibe, Pacific Northwest National Laboratory, USA; Ulrike Meier Yang, Lawrence Livermore National Laboratory, USA

9:35-9:55 Lessons from Running Open Source Projects: Building Sustainable Software and Sustainable Communities

Wolfgang Bangerth, Colorado State University, USA; Timo Heister, Clemson University, USA

10:00-10:20 Data Skills and Software Training to Enable Data-Driven Discovery

Tracy K. Teal, Data Carpentry, USA

10:25-10:45 The Research Software Engineer: An Emerging New Role in Academia in the UK

James Hetherington, University College of London, United Kingdom; Simon Hettrick, University of Sheffield, United Kingdom; Rob Haines, University of Manchester, United Kingdom; Mike Croucher, University of Sheffield, United Kingdom; Alyss Brett, Culham Centre For Fusion Energy, United Kingdom

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Wednesday, March 1

MS145

Reduced Order Modeling Techniques in Large Scale & Data-Driven PDE Problems - Part I of II

9:10 AM-10:50 AM

Room:205

For Part 2 see MS172

A growing number of applications in engineering merge mathematical models built on partial differential equations and complex data (possibly high-dimensional and/or affected by uncertainty) in order to perform tasks such as driving a system to a desired target, ensuring minimal operational risk, identifying unknown or uncertain features or efficiently exploring different scenarios. Data assimilation and uncertainty quantification problems, as well as multiscale and/or multiphysics problems, are currently open challenges for reduced order modeling techniques: whilst making the solution of these many-query, and potentially large- scale, problems computationally tractable, many outstanding theoretical and algorithmic challenges remain. The goal of this minisymposium is to bring together researchers who are active in the aforementioned fields, to present novel and promising methods, and to discuss future trends for research in the field of reduced order modeling.

Organizer: Andrea Manzoni
École Polytechnique Fédérale de Lausanne, Switzerland

Organizer: Matthew J. Zahr
Stanford University, USA

9:10-9:30 Online Interpolation Point Refinement for Reduced Order Models

Nathan Kutz, Syuzanna Sargsyan, and Krithika Manohar, University of Washington, USA; Steven Brunton, Princeton University, USA

continued on next page

Wednesday, March 1

MS145

Reduced Order Modeling Techniques in Large Scale & Data-Driven PDE Problems - Part I of II

9:10 AM-10:50 AM

continued

9:35-9:55 Multifidelity Monte Carlo Estimation of Variances and Sensitivity Indices

Elizabeth Qian, Massachusetts Institute of Technology, USA; Dan O'Malley, Los Alamos National Laboratory, USA; Benjamin Peherstorfer, Massachusetts Institute of Technology, USA; Velimir V. Vesselinov, Los Alamos National Laboratory, USA; Karen E. Willcox, Massachusetts Institute of Technology, USA

10:00-10:20 Nonlinear Model Order Reduction for Steady Aerodynamic Design Applications

Kyle Washabaugh, Matthew J. Zahr, and Charbel Farhat, Stanford University, USA

10:25-10:45 Multi Space Reduced Basis (MSRB) Preconditioners for Large-Scale Parametrized PDEs

Niccolò Dal Santo, Andrea Manzoni, Simone Deparis, and Alfio Quarteroni, École Polytechnique Fédérale de Lausanne, Switzerland

Wednesday, March 1

MS146

Novel Numerical Methods for Maxwell's Equations and Magnetohydrodynamics - Part I of II

9:10 AM-10:50 AM

Room:206

For Part 2 see MS173

Maxwell's equations describe how electric and magnetic fields interact. Magnetohydrodynamics (MHD) models the magnetic properties of electrically conducting fluids. Both involve fundamental and important systems of partial differential equations that have wide range of applications such as fusion, astrophysical phenomena, and electromagnetic materials. The main theme of the minisymposium is on the advanced numerical methods for solving these types of models. The focus is on robust temporal and spatial discretizations, efficient nonlinear and linear solvers, and practical implementations for a wide range of applications related to Maxwell's equations and the MHD model.

Organizer: Xiaozhe Hu
Tufts University, USA

Organizer: James H. Adler
Tufts University, USA

9:10-9:30 A Least-Squares Approach to Two-Fluid, Electromagnetic Plasma

Thomas Manteuffel and Chris Leibs, University of Colorado Boulder, USA

9:35-9:55 Vector-Potential Finite-Element Formulations for Two-Dimensional Resistive Magnetohydrodynamics

Yunhui He, Memorial University, Newfoundland, Canada

10:00-10:20 Regionally Implicit and Explicit Methods for the Relativistic Vlasov-Maxwell System

Pierson Guthrey, Iowa State University, USA

10:25-10:45 A Fast Linear-Time Higher-Order Unconditionally Stable 2D Implicit Wave Equation Solver

Thavappiragasam Mathialakan, Aditya Viswanathan, and Andrew J. Christlieb, Michigan State University, USA

Wednesday, March 1

MS147

Advances in Computational Fractional PDEs - Part I of II

9:10 AM-10:50 AM

Room:209

For Part 2 see MS174

Development of highly efficient and accurate computational methods for fractional PDEs is a challenging area due to the nonlocality of the derivative terms. This requires special treatment of the fractional derivatives while maintain higher order of accuracy. Fractional models are considered heavily to account for anomalous diffusion and dispersion that takes place in many applications. Designing effective schemes based on FD, FEM, and spectral methods, by utilizing special time integrators, and stochastic simulation, create serious challenges for efficient and fast algorithms. The minisymposium will report the recent advances in the computational methods for deterministic and stochastic fractional models. The talks in this minisymposium will present a broad range of tools, methods, venues, problems, and applications.

Organizer: Abdul Khaliq
Middle Tennessee State University, USA

Organizer: Khaled Furati
King Fahd University of Petroleum and Minerals, Saudi Arabia

Organizer: Mohsen Zayernouri
Michigan State University, USA

9:10-9:30 Fourth Order Time Stepping Methods for Space Fractional Nonlinear Schrodinger Equations

Abdul M. Khaliq, Middle Tennessee State University, USA

9:35-9:55 Sparse Approximation of Stochastic Tempered Fractional Differential Equations

Guang Lin, Purdue University, USA

10:00-10:20 A Unified Spectral Method for Time and Space Distributed FPDEs

Ehsan Kharazmi and Mohsen Zayernouri, Michigan State University, USA

10:25-10:45 Numerical Solution of Fractional Partial Differential Equations Via Hybrid Functions

Somayeh Mashayekhi, Florida State University, USA

Wednesday, March 1

MS148

Taming the Beast: Broadening the Applicability of Algebraic Multigrid - Part I of II

9:10 AM-10:50 AM

Room:210

For Part 2 see MS175

In theory, everything works in practice. In practice, algebraic multigrid (AMG) can be a sensitive method. For certain classes of problems, AMG has proven to be a fast and scalable solver for large, sparse linear systems. However, AMG can be less robust when extended to more general systems than well-behaved M-matrices. In this minisymposium, theoretical observations are used to motivate practical AMG methods that broaden the applicability of AMG. Convergence theory for AMG is discussed, along with the optimal interpolation operator with respect to two-grid convergence. Practical ways of achieving theoretical convergence and approximating such an operator are presented, with numerical results from a wide class of problems resulting from the discretization of partial differential equations (PDEs). Convergence theory is connected with PDE discretization by considering how to efficiently achieve full-multigrid like behavior, i.e. achieve discretization accuracy, in an AMG algorithm, and methods to reduce communication in the parallel setting are presented. AMG is also extended to linear systems resulting from the study of graph Laplacians for undirected, directed, and signed graphs, associated with large, scale-free data networks.

Organizer: Ben Southworth

University of Colorado Boulder, USA

9:10-9:30 Algebraic Multigrid: Theory and Practice

James Brannick, Pennsylvania State University, USA; Karsten Kahl, Bergische Universität Wuppertal, Germany

9:35-9:55 Improved Robustness with Root-Node Algebraic Multigrid

Luke Olson, University of Illinois at Urbana-Champaign, USA; Thomas Manteuffel, University of Colorado Boulder, USA; Jacob B. Schroder, Lawrence Livermore National Laboratory, USA; Ben Southworth, University of Colorado Boulder, USA

10:00-10:20 Algebraic Multigrid for Non-Symmetric Linear Systems

Ben Southworth, Thomas Manteuffel, and John Ruge, University of Colorado Boulder, USA

10:25-10:45 Discretization-Accuracy Convergence for Full Algebraic Multigrid

Wayne Mitchell and Steve McCormick, University of Colorado Boulder, USA; Robert D. Falgout, Lawrence Livermore National Laboratory, USA; Thomas Manteuffel, University of Colorado Boulder, USA

continued in next column

Wednesday, March 1

MS149

Liquid Crystals and Related Models, Computation, and Applications - Part I of II

9:10 AM-10:50 AM

Room:211

For Part 2 see MS176

Liquid crystals are a work-horse technology in industry (e.g. for electronic displays). But there are many other potential technological uses of liquid crystals, such as in material design. In addition, liquid crystal models find use in modeling "active matter" systems. Therefore, new methods are needed to model, analyze, simulate, and control these systems. This minisymposium will deliver a range of talks on modeling/theory, numerical analysis, and applications related to liquid crystals.

Organizer: Shawn W. Walker

Louisiana State University, USA

Organizer: Noel J. Walkington

Carnegie Mellon University, USA

Organizer: Amanda E. Diegel

Louisiana State University, USA

9:10-9:30 Finite Element Approximation of Nematic Liquid Crystals with Variable Degree of Orientation

Wujun Zhang, University of Maryland, USA; Ricardo Nochetto, University of Maryland, College Park, USA; Shawn W. Walker, Louisiana State University, USA

9:35-9:55 A Finite Element Scheme for a Phase Field Model of Nematic Liquid Crystals

Amanda E. Diegel and Shawn W. Walker, Louisiana State University, USA

10:00-10:20 Weak Free Surface Anchoring Model for Partially Wetting Nanoscale Nematic Liquid Films

Michael A. Lam and Linda Cummings, New Jersey Institute of Technology, USA; Te-Sheng Lin, National Chiao Tung University, Taiwan; Lou Kondic, New Jersey Institute of Technology, USA

10:25-10:45 Biological Plywoods

Alejandro D. Rey, McGill University, Canada

Wednesday, March 1

MS150

Innovative Algorithms for Eigenvalue and Singular Value Decomposition - Part I of II

9:10 AM-10:50 AM

Room:212

For Part 2 see MS177

The minisymposium will focuses on the first steps taken on the development of novel software methodologies and algorithm for the next generation of HPC systems. Some scale challenges will be addressed; the goal is to close the "application-architecture peak performance gap" by exploring algorithms and runtime improvements that will enable key science applications to better exploit the architectural features of the extreme-scale systems. The contributed talks will cover new approaches that can overcome the limitations of existing dense/sparse eigensolver libraries on platforms that require fine granularity and memory-aware computational tasks combined with asynchronism in parallel execution.

Organizer: Azzam Haidar

University of Tennessee, USA

9:10-9:30 Toward Distributed Eigenvalue and Singular Value Solver Using Data Flow System

Azzam Haidar, University of Tennessee, USA; Aurelien Bouteiller, George Bosilca, and Stanimire Tomov, University of Tennessee, Knoxville, USA; Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA

9:35-9:55 Towards Materials Design with Extreme-Scale Quantum Simulations

Raffaele Solcà, Anton Kozhevnikov, Thomas C. Schulthess, and Thomas C. Schulthess, ETH Zürich, Switzerland

10:00-10:20 Communication Avoiding and Synchronous Reducing Techniques for Dense Parallel Eigenvalue Solver

Toshiyuki Imamura and Yusuke Hirota, RIKEN Advanced Institute for Computational Science, Japan; Susumu Yamada and Masahiko Machida, Japan Atomic Energy Agency, Japan

10:25-10:45 Computing a Partial SVD of General Matrices

Osni A. Marques, Lawrence Berkeley National Laboratory, USA

Wednesday, March 1

MS151

Collocation Methods for High-Dimensional Parameterized Problems in Uncertainty Quantification - Part I of II

9:10 AM-10:50 AM

Room:213

For Part 2 see MS178

Many problems in uncertainty quantification rely on robust and efficient parametric collocation approximations. Collocation methods are attractive because they are simple, non-intrusive, and are flexible enough to exploit structure such as smoothness, sparsity, low-rank manifolds, or low intrinsic-dimensionality. The current challenges that this minisymposium aims to address involve quasi-optimal distributions for approximation, robust quadrature, dimensional scaling, measure adaptivity, and Bayesian inference. This minisymposium bring together researchers from across the applied and computational mathematics community to discuss and collaborate on novel theoretical and computational advances in collocation strategies, and to discuss future directions for research.

Organizer: John D. Jakeman

Sandia National Laboratories, USA

9:10-9:30 Multivariate Quadrature Rules for Correlated Random Variables

John D. Jakeman, Sandia National Laboratories, USA; Akil Narayan, University of Utah, USA

9:35-9:55 Gradient-Enhanced Stochastic Collocation Methods for Uncertainty Quantification

Ling Guo, Shanghai Normal University, China; Akil Narayan, University of Utah, USA; Dongbin Xiu, Ohio State University, USA; *Tao Zhou,* Chinese Academy of Sciences, China

continued in next column

10:00-10:20 Stochastic Collocation Methods Via Compressive Sensing and Its Applications in Uncertainty Quantification

Ling Guo, Shanghai Normal University, China; Akil Narayan, University of Utah, USA; Yuhang Chen, Ohio State University, USA; Tao Zhou, Chinese Academy of Sciences, China; Dongbin Xiu, Ohio State University, USA

10:25-10:45 Effective Quadratures: Least Squares Polynomials for Parametric Studies

Pranay Seshadri, Cambridge University, United Kingdom; Akil Narayan, University of Utah, USA

Wednesday, March 1

MS152

Non-Destructive Testing and Interior Transmission Eigenvalues

9:10 AM-10:50 AM

Room:214

The aim in non-destructive testing is to visualize the interior of a given three-dimensional object in order to uncover location, size, and geometry of inhomogeneities. Interior transmission eigenvalues can be used for this purpose. However the efficient numerical calculation of those is a challenging task due to the fact that the corresponding interior transmission problem is neither elliptic nor self-adjoint. The goal of this minisymposium is to highlight new developments. It aims to bring together mathematicians and scientists working on these methods to share new results and exchange ideas.

Organizer: Andreas Kleefeld

Jülich Supercomputing Centre, Germany

9:10-9:30 An Introduction to Interior Transmission Eigenvalues and Non-Destructive Testing

Andreas Kleefeld, Jülich Supercomputing Centre, Germany

9:35-9:55 A Spectrum Projection Method for Transmission Eigenvalues

Jiguang Sun, Michigan Technological University, USA

10:00-10:20 Spectral Results of the Interior Transmission Eigenvalues for Maxwell's Equations

Shixu Meng, University of Delaware, USA; Houssem Haddar, CMAP, Ecole Polytechnique, France

10:25-10:45 Homogenization of the Transmission Eigenvalue Problem for a Periodic Media

Isaac Harris, Texas A&M University, USA

Wednesday, March 1

MS153

Invariant Domain and Asymptotic Preserving Techniques for Hyperbolic Systems - Part I of II

9:10 AM-10:25 AM

Room:215

For Part 2 see MS180

Positive density and internal energy are invariant properties for the Euler equations; likewise, positive water height is an invariant property of the shallow water equations. Many first-order methods are known to be invariant-domain preserving, but extending theses techniques to higher-order is non-trivial. The difficulty consists of being invariant, high-order accurate and to satisfy enough entropy inequalities for the approximation to converge to an entropy solution. Invariant-domain preserving are important in applications where being 'in bounds' is essential. The objective of minisymposium is to gather specialists to present the latest developments on invariant-domain preserving methods for the approximation of hyperbolic systems.

Organizer: Jean-Luc Guermond

Texas A &M University, USA

9:10-9:30 Numerical Methods for the Chemotaxis Models

Yekaterina Epshteyn, University of Utah, USA

9:35-9:55 Title Not Available at Time of Publication

Christophe Berthon, Université de Nantes, France

10:00-10:20 Convergence Estimates for the Approximation of Scalar Conservation Equations

Bojan Popov, Texas A&M University, USA

Wednesday, March 1

MS154

Flooding the Cores - Computing Flooding Events on Modern Architectures - Part I of II

9:10 AM-10:50 AM

Room:216

For Part 2 see MS181

Detailed simulation of flooding events, such as storm surges, tsunamis or overland floods, requires substantial computing power. Supercomputing technology today is characterized by an increasing amount of parallelism on all scales. Hence, numerical methods, algorithms and software need to be tuned for data parallelism, multi- and many-core compute nodes (including accelerator technology) and large-scale parallelism. This minisymposium thus focuses on how to literally flood the cores with simulation tasks. We will discuss approaches to reduce time to solution for simulating complex flooding events on supercomputers and architectures characterized by many-core and accelerator technologies, including GPUs and Xeon Phis.

Organizer: Michael Bader

Technische Universität München, Germany

Organizer: Tobias Weinzierl

Durham University, United Kingdom

Organizer: Kyle T. Mandli

Columbia University, USA

9:10-9:30 Requirements and Progress Towards Answering the Big Questions in Storm Surge Modelling

Kyle T. Mandli, Colton Conroy, and Jiao Li, Columbia University, USA

9:35-9:55 Computational Efficiency of a Parallel High-Order Spectral Method for 3D Water Wave Simulations

Nicole Beisiegel and Frédéric Dias, University College Dublin, Ireland

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Wednesday, March 1

MS154

Flooding the Cores - Computing Flooding Events on Modern Architectures - Part I of II

9:10 AM-10:50 AM

continued

10:00-10:20 Multiscale Flood Simulations in Urban Regions

Christoph M. Ertl, Florian Mintgen, Nevena Perovic, Hao Zeng, Michael Manhart, and *Ralf-Peter Mundani*, Technische Universität München, Germany

10:25-10:45 Scaling at Exascale in Blended Isogeometric, Discontinuous Galerkin, and Particle-in-Cell Approaches

Craig Michoski, Robert D. Moser, and Clint Dawson, University of Texas at Austin, USA; Varis Carey, University of Colorado at Denver, USA; Chris Simmons, University of Texas at Austin, USA

Wednesday, March 1

MS155

Challenges and Approaches for Enabling Large-Scale Molecular Simulation - Part I of II

9:10 AM-10:50 AM

Room:217

For Part 2 see MS182

Molecular simulation is a powerful technique to investigate chemical/biological processes, and materials properties. Molecular dynamics (MD) simulations are characterized by a force field, involving many parameters to describe the interactions between atoms. Accurately accounting for these interactions constrains the timestep lengths in MD simulations to femtoseconds, while several chemical or biological processes of interest take place in the span of seconds and beyond. Today, state of the art simulations on general purpose computers are way behind this target. While the significantly improved computational power of modern clusters provide an exciting opportunity, important challenges need to be addressed to fully leverage the potential of today's processors and accelerators in MD simulations. First and foremost, parallelism at each level (vector processing, shared memory and distributed memory) must be exploited to obtain the best absolute performance. Novel numerical methods, better integrators and enhanced sampling techniques can complement parallelism to significantly improve the temporal span of MD simulations. Finally, solutions must be portable across different architectures and the large variety of molecular force fields actively used in the community. This minisymposium brings together experts to explore potential solutions across the spectrum of challenges faced by the molecular simulation community.

continued in next column

Organizer: H. Metin Aktulga
Michigan State University, USA

Organizer: William J. Mcdoniel
RWTH Aachen University, Germany

9:10-9:30 Fast Charge Equilibration Solvers for Polarizable Force Fields

H. Metin Aktulga and Kurt O'Hearn, Michigan State University, USA

9:35-9:55 Performance Issues for Modeling Materials via Molecular Dynamics on Current and Future Hardware

Steve Plimpton, Sandia National Laboratories, USA; Mike Brown, Intel Corporation, USA; Stan Moore and Christian Trott, Sandia National Laboratories, USA

10:00-10:20 Scalable, Reproducible and Fast Quantum and Reactive Molecular Dynamics Simulations

Aiichiro Nakano and Rajiv K. Kalia, University of Southern California, USA; Fuyuki Shimojo, Kumamoto University, Japan; Priya Vashishta, University of Southern California, USA

10:25-10:45 Greatly Scalable Multiple-Copy Enhanced Sampling Algorithm on Massively Parallel Computing

Wei Jiang, Argonne National Laboratory, USA

Wednesday, March 1

MS156

Understanding Performance Variability Due to Application-Data Center Interaction - Part I of II

9:10 AM-10:50 AM

Room:218

For Part 2 see MS183

System issues and applications' contention for resources can adversely impact system efficiency and application runtimes resulting in large performance variability. Attributing performance issues to specific root causes, and quantifying the impact under production conditions are difficult. Recent advances in platform and application instrumentation, along with data analytics and visualization techniques for high-volume, multi-dimensional data, can provide the basis for such evaluations. This minisymposium brings together experts in these areas to discuss current techniques and progress in detection, understanding, and attribution of system and application performance issues and how such insight is being used to improve application performance and system operations.

Organizer: James Brandt

Sandia National Laboratories, USA

Organizer: Ann Gentile

Sandia National Laboratories, USA

Organizer: Abhinav Bhatele

Lawrence Livermore National Laboratory, USA

Organizer: Todd Gamblin

Lawrence Livermore National Laboratory, USA

9:10-9:30 Network Congestion: Challenges and Approaches to Understanding Application Impact

Ann Gentile, James Brandt, Anthony Agelastos, and Benjamin Allan, Sandia National Laboratories, USA

9:35-9:55 Detecting Application Interference Through System Log Analysis with Spark

Diana Moise, Cray, Inc., USA

10:00-10:20 Analysis of User Job Level Performance Data Using XDMoD with Application Kernels

Thomas Furlani, State University of New York at Buffalo, USA

10:25-10:45 Monitoring HPC Systems for Improving Efficiency

Ayse Coskun, Boston University, USA

continued in next column

Wednesday, March 1

MS157

Advances in Dynamic Graphs: Algorithms, Applications and Challenges - Part I of II

9:10 AM-10:50 AM

Room:219

For Part 2 see MS184

Many interesting phenomena can be modeled as dynamic graphs. For example, in biology, complex interactions of microbes evolve over a period of time; in cybersecurity, malicious activities evolve over a period of time through complex interactions with the system; and in transportation networks, dynamic analysis of traffic is essential for modeling evacuation plans and contingency measures. Several graph algorithms such as dynamic community detection, network alignment, graph matching and edge cover formulations play a vital role in the study of real-world dynamic networks. The goal of this minisymposium is to bring together computational researchers and domain experts exploring dynamic graph models, algorithms, and applications of interest. We propose a two-part minisymposium covering problems from application domains in biology (microbial communities, brain networks), cybersecurity (anomaly detection, control systems), and transportation networks. These talks will be augmented with talks on dynamic graph algorithmic modeling, design and development at scale.

Organizer: Ananth Kalyanaraman

Washington State University, USA

Organizer: Mahantesh Halappanavar

Pacific Northwest National Laboratory, USA

continued on next page

Wednesday, March 1

MS157

Advances in Dynamic Graphs: Algorithms, Applications and Challenges - Part I of II

9:10 AM-10:50 AM

continued

9:10-9:30 Advances in Algorithms and Applications for Dynamic Graphs

Ananth Kalyanaraman, Washington State University, USA; Mahantesh Halappanavar, Pacific Northwest National Laboratory, USA

9:35-9:55 Dynamic Networks of Microbial Biofilms

Radu Marculescu and Chieh Lo, Carnegie Mellon University, USA

10:00-10:20 Dynamic Brain Networks

Kristian Eschenberg, Tom Grabowski, and David Haynor, University of Washington, USA

10:25-10:45 Quantitative Assessment of Transportation Network Vulnerability with Dynamic Traffic Simulation Methods

Venkateswaran Shekar, University of Massachusetts, Dartmouth, USA; *Samrat Chatterjee* and Mahantesh Halappanavar, Pacific Northwest National Laboratory, USA; Lance Fiondella, University of Massachusetts, Dartmouth, USA

Wednesday, March 1

MS158

Multi-Fidelity and Multi-Information-Source Methods - Part I of II

9:10 AM-10:50 AM

Room:220

For Part 2 see MS185

Analysis and decision-making processes for complex, multidisciplinary systems often begin with low-fidelity models and progressively incorporate higher fidelity tools. In many cases, however, there is not just a set of computational models clearly ranked in terms of fidelity. Rather, there are multiple models with different types of distortion of the true system. Moreover often the analysis and decision involve other information sources (e.g., expert opinion, experiments). Typically, these different information sources are combined in an ad hoc manner. This minisymposium features research that is developing principled approaches that explicitly integrate the breadth of available information sources.

Organizer: Karen E. Willcox

Massachusetts Institute of Technology, USA

9:10-9:30 A Bayesian Approach to Optimal Coupling of Multidisciplinary Models

Ricardo Baptista, Youssef M. Marzouk, Benjamin Peherstorfer, and Karen E. Willcox, Massachusetts Institute of Technology, USA

9:35-9:55 Multi-Information Source Optimization with Unknown Constraints

Matthias Poloczek and Peter I. Frazier, Cornell University, USA

10:00-10:20 Reducing the Error of Monte Carlo Algorithms by Learning Control Variates

David Wolpert, Santa Fe Institute, USA; Brendan Tracey, Santa Fe Institute and Massachusetts Institute of Technology, USA

10:25-10:45 A Model Reification Approach to Fusing Information from Multifidelity Information Sources

Doug Allaire and William Thomison, Texas A&M University, USA

Wednesday, March 1

MS159

Bridging Macrophysics and Microphysics in Kinetic Plasma Models: Computational Perspectives - Part I of II

9:10 AM-10:50 AM

Room:Crystal AF - 1st Fl

For Part 2 see MS186

Including the microscopic physics in macroscopic computer simulations of magnetized plasmas is a very challenging task since mathematical models, e.g., the Vlasov-Maxwell equations, are relatively highly dimensional, strongly non-linear and extremely multiscale. The strong interest on applications as magnetic fusion energy and astrophysical plasmas and the super-computing architectures available nowadays and in the forthcoming future (from peta-scale to exa-scale computers) are driving the development of new robust and efficient computational approaches and models. This minisymposium aims at gathering researchers and experts in multiscale computational modelling of plasma physics problems, innovative numerical techniques and high performance computing for large-scale computer simulations.

Organizer: Gian Luca Delzanno

Los Alamos National Laboratory, USA

Organizer: Gianmarco Manzini

Los Alamos National Laboratory, USA

9:10-9:30 Spectral Methods for Multiscale Plasma Physics Simulations

Gian Luca Delzanno and Gianmarco Manzini, Los Alamos National Laboratory, USA; Juris Vencels and Stefano Markidis, KTH Royal Institute of Technology, Sweden; Vadim Roytershteyn, Space Science Institute, USA

continued on next page

9:35-9:55 Hybrid Method and Its Applications to Selected Problems in Space Physics
Vadim Roytershteyn, Space Science Institute, USA

10:00-10:20 A Multiscale, Coulomb Collision Machine-Learning Approach for Particle-in-Cell Plasma Algorithms
Luis Chacon and Guangye Chen, Los Alamos National Laboratory, USA

10:25-10:45 Fluid-Kinetic Coupling with the Hermite-Fourier Spectral Method
Stefano Markidis, KTH Royal Institute of Technology, Sweden; Gian Luca Delzanno and Gianmarco Manzini, Los Alamos National Laboratory, USA; Ivy Bo Peng and Erwin Laure, KTH Royal Institute of Technology, Sweden

Wednesday, March 1

MS160

Fast Solvers for Large-Scale Inverse Problems in Imaging - Part I of II

9:10 AM-10:50 AM

Room:Crystal CD - 1st Fl

For Part 2 see MS187

We discuss recent advances in algorithms for large-scale inverse problems in the imaging sciences. Due to ill-conditioning, non-convexity, large-problem size, infinite-dimensional structure, and the need for adjoint operators, such problems are challenging to solve. Key algorithmic challenges include computational complexity, memory consumption, a vast number unknowns as well as model and data uncertainties. We showcase state-of-the-art techniques in scientific computing to tackle these challenges.

Organizer: Andreas Mang
University of Texas at Austin, USA

Organizer: George Biros
University of Texas at Austin, USA

9:10-9:30 Mathematical Models for the Correspondence Problem
Jan Modersitzki, University of Lübeck, Germany

9:35-9:55 A Lagrangian Solver for Diffeomorphic Image Registration
Lars Ruthotto, Emory University, USA; Andreas Mang, University of Texas at Austin, USA

10:00-10:20 Reduced Order Models for One-Step Multispectral Quantitative Photoacoustic Tomography
Arvind Saibaba, North Carolina State University, USA; *Sarah Vallelian*, Statistical and Applied Mathematical Sciences Institute, USA

10:25-10:45 Stochastic Newton and Quasi-Newton Methods for Large-Scale Least-Squares Problems
Julianne Chung, Matthias Chung, and *Joseph T. Slagel*, Virginia Tech, USA; Luis Tenorio, Colorado School of Mines, USA

Wednesday, March 1

MS161

Reduced Order Models for Fluids: Achievements and Open Problems - Part I of II

9:10 AM-10:50 AM

Room:301

For Part 2 see MS188

This minisymposium aims at giving a survey of recent developments in the reduced order modeling of fluid flows. Computational modeling, numerical analysis and applications to realistic engineering and geophysical flow problems will be covered in this minisymposium. Both achievements and open problems in the reduced order modeling of fluid flows will be discussed.

Organizer: Jeff Borggaard
Virginia Tech, USA

Organizer: Lizette Zietsman
Virginia Tech, USA

9:10-9:30 Hierarchical Model Reduction Methods for Incompressible Navier-Stokes Equations in Pipes and Networks: Challenges and Perspectives
Alessandro Veneziani, Emory University, USA

9:35-9:55 Adaptive Reduced-Order Modeling for Flows under Uncertainty
Sebastian Ullmann and Jens Lang, Technische Universität Darmstadt, Germany

10:00-10:20 libROM: A Distributed-Memory Adaptive Incremental Proper Orthogonal Decomposition
Geoffrey M. Oxberry, Bill Arrighi, Tanya Kostova-Vassilevska, and Robert W. Anderson, Lawrence Livermore National Laboratory, USA

10:25-10:45 The Effect of Snapshot Divergence Error on the Accuracy of Reduced Order Modeling
Muhammad Mohebujjaman and Leo Rebholz, Clemson University, USA; Traian Iliescu and Xuping Xie, Virginia Tech, USA

Wednesday, March 1

MS162

Model Reduction for Optimal Control Problems: Perspectives from Junior Researchers - Part I of II

9:10 AM-10:50 AM

Room:302

For Part 2 see MS189

Optimization and control of systems governed by partial differential equations usually requires expensive evaluations of the forward problem or the optimality system. In a time-critical application such as control, this is often prohibitive, and model reduction can circumvent that problem. In the proposed session, junior researchers such as Ph.D students and PostDocs will present various approaches to model reduction in the context of control. We will consider nonlinear optimization, high-dimensional parameter spaces and feedback control and a variety of applications.

Organizer: Alessandro Alla

Florida State University, USA

9:10-9:30 Ghosts of Model Reduction: Past, Present and Yet-To-Come

Christian Himpe and Sara Grundel, Peter Benner, Max Planck Institute for Dynamics of Complex Technical Systems, Germany

9:35-9:55 Solution of Large-Scale Constrained Riccati Equations for Low-Order Models and Controllers of Flows

Jan Heiland, Max Planck Institute, Magdeburg, Germany

10:00-10:20 Feedback Control for Parametric PDEs Using RB Methods

Andreas Schmidt and Bernard Haasdonk, Universität Stuttgart, Germany

10:25-10:45 Reduced-Order Optimal Feedback Control of Semilinear Parabolic Dynamics

Dante Kalise, Radon Institute for Computational and Applied Mathematics, Austria; Karl Kunisch, Universität Graz, Austria

Wednesday, March 1

MS163

Data-Driven Fractional PDE Modeling, Simulation and Prediction - Part I of II

9:10 AM-10:50 AM

Room:303

For Part 2 see MS190

Fractional partial differential equations (FPDEs) are emerging as a powerful tool for modeling challenging multiscale phenomena including overlapping microscopic and macroscopic scales, anomalous transport, and long range time memory or spatial interactions. Compared to integer-order PDEs, the fractional order of the derivatives in FPDEs may be a function of space and time or even a distribution, opening up great opportunities for modeling and simulation of multiphysics phenomena, e.g. seamless transition from wave propagation to difusion, or from local to non-local dynamics. In addition, data-driven fractional differential operators may be constructed to data fit from a particular experiment or specific phenomenon, including the effect of uncertainties, in which the fractional orders are determined directly from the data, and introducing nonlinearities leading to more complex operators, with one or more fractional orders, capable to model less typical phenomena (such as, for instance, wave propagation in heterogeneous systems). This minisymposium will address FPDE modeling, simulation and prediction and their applications.

Organizer: Hong Wang

University of South Carolina, USA

Organizer: George Em Karniadakis

Brown University, USA

9:10-9:30 Analysis and Approximation of a Fractional Cahn-Hilliard Equation

Mark Ainsworth and Zhiping Mao, Brown University, USA

continued in next column

9:35-9:55 Thermodynamically Viable Fractional Wave Equations for Power Law Attenuation in Viscoelastic Media

Sverre Holm, University of Oslo, Norway

10:00-10:20 Space-Time Duality and Anomalous Diffusion

Jim Kelly, Michigan State University, USA

10:25-10:45 Implicit-Explicit Difference Schemes for Fractional Differential Equations with Non-Smooth Solutions

Wanrong Cao, Southeast University, China; Fanhai Zeng, Brown University, USA; Zhongqiang Zhang, Worcester Polytechnic Institute, USA; George Em Karniadakis, Brown University, USA

Wednesday, March 1

MS164

Recent Advances on Numerical Methods and Applications of Phase-Field Methods - Part I of II

9:10 AM-10:50 AM

Room:304

For Part 2 see MS191

Interfacial dynamics in complex fluids presents tremendous challenges to science. From a fluid mechanical viewpoint, the essential physics is the coupling between interfacial movement and the flow of the bulk fluids. Phase field (diffuse-interface) methods start from a multi-scale point of view and treat the interface as a microscopic transition zone of small but finite width. Then a set of governing equations can be derived that are thermodynamically consistent and mathematically well-posed. This principle is very powerful and flexible. It has been applied successfully to describe complicated interfaces in various complex fluids. Well designed numerical methods with the diffuse-interface approach can be highly robust and accurate, as long as the interface is well resolved. Phase field methods are now widely used in many branches of science and engineering, such as the material science, biomedical science, biology, chemical engineering. This minisymposium will bring together numerical analysts and computational scientists working on phase field methods to present their recent advances in algorithm designs and applications of phase field methods. The main purposes of this minisymposium are to review the current status, identify problems and future directions, and to promote phase field methods to a wider scientific and engineering community.

Organizer: Xiaofeng Yang
University of South Carolina, USA

Organizer: Jie Shen
Purdue University, USA

9:10-9:30 Incompressible Two-Phase Flows with Open/Outflow Boundaries: Boundary Conditions and Algorithm

Suchuan Dong, Purdue University, USA

9:35-9:55 Scalable Compact Localized Exponential Time Differencing Method for Simulating Coarsening Dynamics of Cahn-Hilliard Equations

Lili Ju, University of South Carolina, USA

10:00-10:20 Computational Models of the Endoplasmic Reticulum, Bifurcation and Evolution

Keith Promislov, Michigan State University, USA

10:25-10:45 Linear Unconditional Energy-Stable Splitting Schemes for Mixtures of Nematic-Isotropic Flows with Anchoring Effects

Giordano Tierra, Temple University, USA

continued in next column

Wednesday, March 1

MS165

Efficient Algorithms for Bayesian Inverse Problems Governed by PDE Forward Problems - Part I of II

9:10 AM-10:50 AM

Room:305

For Part 2 see MS192

Inverse problems arise when we seek to determine unknown parameters from observational data and mathematical models that relate the parameters to the data. These problems arise across all areas of science, engineering, medicine, and beyond. Inverse problems are often ill-posed; that is, multiple values of the parameters may be consistent with the data to within the noise. Bayesian inference provides a systematic framework for quantifying the resulting uncertainty in the parameters. However, the Bayesian formulation presents significant challenges. First, the parameter to be inferred is often a spatially correlated field, resulting in a high dimensional parameter space after discretization. Second, the forward model is often computationally expensive to solve, particularly when it takes the form of PDEs. The focus of this minisymposium is on recent advances in algorithms for the Bayesian approach to large-scale PDE constrained inverse problems. Specific emphasis is on methods that address the twin challenges of expensive forward problems and high-dimensional parameter spaces. Recent advances in derivative-informed sampling techniques for Markov Chain Monte Carlo, multilevel and high order Quasi Monte Carlo methods, and dimensionality/data reduction techniques will be presented.

Organizer: Vishwas Hebbur Venkata Subba Rao
Virginia Tech, USA

Organizer: Omar Ghattas
University of Texas at Austin, USA

continued on next page

Wednesday, March 1

MS165

Efficient Algorithms for Bayesian Inverse Problems Governed by PDE Forward Problems - Part I of II

9:10 AM-10:50 AM

continued

Organizer: Umberto Villa
University of Texas at Austin, USA

Organizer: Tan Bui-Thanh
University of Texas at Austin, USA

9:10-9:30 Cluster Sampling Filters for Non-Gaussian Data Assimilation
Ahmed Attia, Virginia Tech, USA

9:35-9:55 Adaptive Dimension Reduction to Accelerate Infinite-Dimensional Geometric MCMC
Shiwei Lan, California Institute of Technology, USA; Mark Girolami and Andrew Stuart, University of Warwick, United Kingdom

10:00-10:20 Optimization-Based Samplers in a Measure Transport Framework
Zheng Wang and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

10:25-10:45 Multilevel Higher Order Quasi Monte Carlo Methods for Bayesian Inverse Problems
Robert N. Gantner, ETH Zürich, Switzerland; Josef Dick and Quoc T. Le Gia, University of New South Wales, Australia; Christoph Schwab, ETH Zürich, Switzerland

Wednesday, March 1

MS166

Computational Methods for Illumination Optics - Part I of II

9:10 AM-10:50 AM

Room:221

For Part 2 see MS193

The objective of this minisymposium is to present advanced numerical methods that can be used in the design of illumination devices. Examples are Monge-Ampere solvers to compute freeform surfaces or numerical schemes for Liouville's equation from geometrical optics to calculate photomeric variables at the target of a non-imaging optical system.

Organizer: Jan Ten Thije Boonkkamp
Eindhoven University of Technology, Netherlands

9:10-9:30 Inverse Reflector Problem in Arbitrary Coordinates
Jan Ten Thije Boonkkamp, Eindhoven University of Technology, Netherlands

9:35-9:55 Monge-Ampère Equation in Freeform Illumination Optics
Rengmao Wu, University of Arizona, USA; Zhenrong Zheng, Zhejiang University, China

10:00-10:20 Numerical Approximation of Optimal Transport Maps via Monge-Ampere Equations
Brittany Froese, New Jersey Institute of Technology, USA

10:25-10:45 Freeform Multifocal Lenses Designed with Supporting Quadric Method (SQM): Geometry and Diffraction Effects
Vladimir Oliker, Emory University, USA

Wednesday, March 1

MS167

Inverse Problems and Robust Uncertainty Estimation with Applications in Science and Engineering - Part I of II

9:10 AM-10:50 AM

Room:222

For Part 2 see MS194

In industrial science and engineering, experimentation is often driven by the need for data to make specific decisions, but the data itself generally does not inform the decision-making process. Using models of how the data is captured or generated to extract the required information from the measurements is applied inverse problems. There has been a significant shift in industry to solve inverse problems statistically, in order to robustly quantify uncertainties or assign levels of confidence, not just to the data or calculations from the data, but to the final decisions themselves. This minisymposium collects some of the latest research on applied and industrial inverse problems as well as advanced statistical methods for solving them, with an eye towards how the statistical analysis of data can drive decision making in applied and industrial environments.

Organizer: Aaron B. Luttman
National Security Technologies, LLC, USA

9:10-9:30 Estimating Particle Size Distributions in Dynamic Experiments via Mie Scattering
Aaron B. Luttman and Marylesa Howard, National Security Technologies, LLC, USA

9:35-9:55 Robust-Adaptive Decision-making for Financial Forecasting
Francois Hemez, Los Alamos National Laboratory, USA

10:00-10:20 Using Conjugate Gradient Iterations for Sampling in Hierarchical Gaussian Inverse Problems
Johnathan M. Bardsley, University of Montana, USA

10:25-10:45 Image Processing, Optimization, and Uncertainty Quantification for Large-Scale Experimental Science
Richard Archibald, Oak Ridge National Laboratory, USA

Wednesday, March 1

CP11

Uncertainty Quantification - Part III of IV

9:10 AM-10:50 AM

Room:223

For Part 2 see CP9
For Part 4 see CP13

Chair: To Be Determined

9:10-9:20 An Efficient Stochastic Quasi-Newton Mcmc Method for Stochastic Inversion of Linear Elasticity Problem Using Kernel Pca, Automatic Differentiation and Adjoint Method

Xiao Chen, Lawrence Livermore National Laboratory, USA; Wenju Zhao, Florida State University, USA; Charanraj Thimmisetty, Joshua A. White, and Charles Tong, Lawrence Livermore National Laboratory, USA

9:22-9:32 High-Dimensional Intrinsic Interpolation Using Gaussian Process Regression

Charanraj Thimmisetty, Lawrence Livermore National Laboratory, USA; Roger Ghanem, University of Southern California, USA; Christina Morency, Xiao Chen, Joshua A. White, and Charles Tong, Lawrence Livermore National Laboratory, USA

9:34-9:44 An Importance Sampling Approach to Risk Estimation

Timur Takhtaganov, Rice University, USA; Drew P. Kouri and Denis Ridzal, Sandia National Laboratories, USA; Matthias Heinkenschloss, Rice University, USA

9:46-9:56 Bayesian Calibration for Parameters of Jwl Equation of State in Cylinder Test

Hua Chen, Haibing Zhou, and Guozhao Liu, Institute of Applied Physics and Computational Mathematics, China; Zhanfeng Sun, Chinese Academy of Engineering Physics (CAEP), China; Shudao Zhang, Institute of Applied Physics and Computational Mathematics, China

continued in next column

9:58-10:08 Bayesian, Multi-Fidelity, Optimization under Uncertainty

Maximilian Koschade and Phaedon S. Koutsourelakis, Technische Universität München, Germany

10:10-10:20 Bayesian Coarse-Graining in Atomistic Simulations: Adaptive Identification of the Dimensionality and Salient Features

Markus Schoeberl, Technische Universität München, Germany; Nicholas Zabaras, University of Notre Dame, USA; Phaedon S. Koutsourelakis, Technische Universität München, Germany

10:22-10:32 A Weighted Kernel PCA-Based Method for Goal-Oriented Optimization and Uncertainty Quantification with Applications to Elastic Parameter Inversion

Charles Talbot, Lawrence Livermore National Laboratory and University of North Carolina at Chapel Hill, USA; Chen Xiao, Charles Tong, and Charanraj Thimmisetty, Lawrence Livermore National Laboratory, USA; Wenju Zhao, Florida State University, USA

10:34-10:44 Method Coupling Harmonic Decomposition and Polynomial Chaos for Seismic Wave Propagation in Uncertain Medium

Pierre Sochala and Florent De Martin, BRGM, France

Wednesday, March 1

CP12

Numerical PDEs - Part III of VI

9:10 AM-10:50 AM

Room:224

For Part 2 see CP10
For Part 4 see CP14

Chair: Prince Chidyagwai, Loyola University, USA

9:10-9:20 Life and Its Many Layers: Eigenfunctions of 1-D Differential Operators with Piecewise Constant Coefficients

Sarah D. Long and James V. Lambers, University of Southern Mississippi, USA

9:22-9:32 Adaptive Methods for Multidimensional Cubature

Fred J. Hickernell, Illinois Institute of Technology, USA

9:34-9:44 Higher Order Numerical Schemes for Non-Conservative Hyperbolic Equations on 2D Unstructured Grids

Julian Koellermeier and Manuel Torrilhon, RWTH Aachen University, Germany

9:46-9:56 Sobolev Discontinuous Galerkin Methods

Adeline Kornelus and Daniel Appelo, University of New Mexico, USA; Thomas M. Hagstrom, Southern Methodist University, USA

9:58-10:08 Monotone Local Projection Stabilization for Nonlinear Hyperbolic Systems

Sibusiso Mabuza, Sandia National Laboratories, USA

10:10-10:20 Dual Least-Squares Finite Element Methods for Hyperbolic Problems

Delyan Z. Kalchev and Thomas Manteuffel, University of Colorado Boulder, USA

10:22-10:32 A Realizability Preserving Discontinuous Galerkin Method for Radiative Transport

Prince Chidyagwai, Loyola University, USA; Florian Scheider, Technische Universität Kaiserslautern, Germany; Benjamin Seibold, Temple University, USA; Martin Frank, RWTH-Aachen, Germany

10:34-10:44 A Godunov-Type Finite-Volume Solver for Nonhydrostatic Euler Equations with a Time-Splitting Approach

Farshid Nazari, and Ram Nair, National Center for Atmospheric Research, USA

Wednesday, March 1

Coffee Break

10:50 AM-11:20 AM

Room:Foyer - 2nd Fl

IP6

Talk Title To Be Announced

11:20 AM-12:05 PM

Room: Grand Ballroom, 2nd Floor

Chair: X. Sherry Li

Lawrence Berkeley National Laboratory, USA

Ann Almgren

Lawrence Berkeley National Laboratory, USA

Lunch Break

12:05 PM-1:30 PM

Attendees on their own

Wednesday, March 1

PD3

Forward Looking Panel

12:15 PM-1:30 PM

Room:Ballroom D - 2nd Fl

Chair: George E. Karniadakis, Brown University, USA

This forward-looking panel will explore the future of CSE in a broad academic context. What new "grand challenges" may drive progress in CSE? How can CSE shape the future of new application fields such as computational medicine and biology, computational geoscience, and materials science? Are there opportunities to extend CSE to new areas such as social network analysis, cybersecurity and the social sciences, with mathematics-based large-scale computing rapidly becoming of crucial importance in almost all areas of society? Is the CSE paradigm and focus sufficiently unique and significant to warrant separate programs, graduate degrees, academic departments, and funding streams?

David Bader

Georgia Institute of Technology, USA

Fariba Fahroo

Air Force Office of Scientific Research, USA

Omar Ghattas

University of Texas at Austin, USA

Horst Simon

Lawrence Berkeley National Laboratory, USA

Karen Willcox

Massachusetts Institute of Technology, USA

Wednesday, March 1

MT6

Exploring the Potential of the PRIMME Eigensolver

1:30 PM-3:10 PM

Room:Ballroom C - 2nd Fl

Chair: Andreas Stathopoulos, College of William & Mary, USA

PRIMME (PReconditioned Iterative MultiMethod Eigensolver) is a high performance library for solving large, sparse Hermitian eigenvalue and singular value problems. Over the last decade, it has acquired a broad user base for high-end and mid-end applications that require the computation of a small number of eigenpairs. Its success lies on its careful implementation of state-of-the-art methods that converge near-optimally even with limited memory. In addition, it offers a host of unique features that are expertly combined and dynamically adjusted to achieve efficiency and robustness. Based on an NSF grant, we have extended the functionality of PRIMME to singular value problems, to more robust computation of interior and larger numbers of eigenpairs, and enhanced with new interfaces to problem solving environments, such as MATLAB and python. This tutorial has three goals. 1. To expose the potential of PRIMME to current and potential users by explaining how and when to enable each functionality, and the behavior of different methods on different problems and computer architectures. 2. To demonstrate how to set up and call the library with example interfaces for MATLAB, PETSc, Trilinos, and python, and with threaded and distributed memory parallelism. 3. To hold a question and answer session with hands-on examples. PRIMME is available at *https://github.com/primme/primme*

Speakers:

Andreas Stathopoulos

College of William & Mary, USA

Eloy Romero

College of William & Mary, USA

Lingfei Wu

IBM T.J. Watson Research Center, USA

Wednesday, March 1

MS168

Probabilistic Machine Learning Tools in Computational Science and Engineering - Part II of II

1:30 PM-3:10 PM

Room:Grand Ballroom - 2nd Fl

For Part 1 see MS140

The never-ending increase of computing power, in combination with the pressing need for robust tools to distill information from data with quantified uncertainty, has put probabilistic machine learning at the epicenter of disruptive developments across many scientific disciplines. Mathematics and engineering in particular, are currently undergoing a steady transition towards which probabilistic data-driven methods come to be viewed as the natural tools to use in computing under uncertainty. This minisymposium invites contributions that showcase the potential of machine learning tools in applied science, including topics in design, uncertainty quantification, inverse problems, and control.

Organizer: Paris Perdikaris

Massachusetts Institute of Technology, USA

Organizer: Ilias Bilionis

Purdue University, USA

1:30-1:50 A Fully Bayesian Solver for ODEs Based on Runge-Kutta

Hans Kersting and Philipp Hennig, Max Planck Institute for Intelligent Systems, Germany

1:55-2:15 Probabilistic Meshless Methods for Partial Differential Equations and Bayesian Inverse Problems

Jon Cockayne, University of Warwick, United Kingdom

2:20-2:40 Solving Multi-Scale Stochastic Partial Differential Equations Using Deep Neural Networks

Ilias Bilionis and Rohit Tripathy, Purdue University, USA

2:45-3:05 Risk-Averse Assessment, Learning, and Optimization Using Surrogate Models

Paris Perdikaris, Massachusetts Institute of Technology, USA; Johannes O. Royset, Naval Postgraduate School, USA

Wednesday, March 1

MS169

Advances in Numerical Methods and Algorithms for Radiation Transport - Part II of II

1:30 PM-3:10 PM

Room:202

For Part 1 see MS142

Radiative transfer and radiation transport modelling play an important role in a variety of physical, chemical, and engineering applications. Due to the equations' large phase space, numerical simulations of transport phenomena are still a formidable challenge in terms of discretization techniques, iterative solution processes, and associated algorithms. This minisymposium intends to bring together researchers from applied mathematics, computational science, physics, and engineering communities to discuss recent advances in computational transport methods (PN, discrete ordinates, Monte-Carlo, iterative approaches) and algorithms for large-scale transport simulations.

Organizer: Jean C. Ragusa

Texas A &M University, USA

1:30-1:50 Rattlesnake - MOOSE-Based Radiation Transport Application for Multi-Physics Simulations at INL

Yaqi Wang, Sebastian Schunert, Mark DeHart, and Richard Martineau, Idaho National Laboratory, USA

1:55-2:15 Fmm Preconditioner for Radiative Transport Equation with Isotropic Coefficients

Yimin Zhong, University of Texas at Austin, USA

2:20-2:40 Goal Oriented Adaptivity Based on the Forward-Adjoint Symmetrization of the Transport Equation

Milan Hanus and Ryan McClarren, Texas A&M University, USA

2:45-3:05 Implicit Solution of the Vlasov-Poisson System

Cory Hauck, Oak Ridge National Laboratory, USA; Charles K. Garrett, Los Alamos National Laboratory, USA

Wednesday, March 1

MS170

Sensitivity Analysis and Uncertainty Quantification of Large-Scale Chaotic Flow Simulations - Part II of II

1:30 PM-2:45 PM

Room:203

For Part 1 see MS143

Chaotic dynamics appears in many scientific and engineering applications. Turbulent fluid flows is a prominent example that attracted significant interest both in science and engineering. Sensitivity analysis of these turbulent and chaotic flow simulations help us understand how the quantities of interest respond to geometry, environmental conditions, simulation parameters, and numerical discretization. Uncertainty quantification of these simulations help us assess the accuracy of quantities predicted by these simulations. Sensitivity analysis and uncertainty quantification has special challenges in chaotic simulations, including turbulent flow simulations, because they are exponentially sensitive to initial condition, and exhibit apparently stochastic behavior. In this minisymposium, the speakers illustrate these challenges and progress in new mathematical techniques developed to overcoming these challenges.

Organizer: Qiqi Wang

Massachusetts Institute of Technology, USA

Organizer: Nicolas R. Gauger

Technische Universität Kaiserslautern, Germany

1:30-1:50 Lyapunov Stability of Scale-Resolving Turbulent Flow Simulations

Pablo Fernandez, Nisha Chandramoorthy, and Qiqi Wang, Massachusetts Institute of Technology, USA

1:55-2:15 Lyapunov Spectrum Shift of an LES from Addition of Localized Aritificial Viscosity

Chaitanya Talnikar and Qiqi Wang, Massachusetts Institute of Technology, USA

2:20-2:40 Exploring Model-Form Uncertainties in Boyancy-Driven Les Simulations

Stefan P. Domino, Sandia National Laboratories, USA

Wednesday, March 1

MS171

Software Productivity and Sustainability for CSE and Data Science - Part II of II

1:30 PM-3:10 PM

Room:204

For Part 1 see MS144

Software is the key crosscutting technology that connects advances in mathematics, computer science, and domain-specific science and engineering to achieve robust simulations and analysis for predictive science, engineering, and other research fields. While software is becoming more complex due to multiphysics and multiscale modeling, the coupling of data analytics, and disruptive changes in computer hardware (due to increases in typical system scale and heterogeneity, including GPUs and additional alternative architectures), software itself has not traditionally received focused attention in the CSE community or been rewarded by that community. The speakers in this minisymposium will discuss work that addresses growing technical and social challenges in software productivity, quality, and sustainability, and thereby is helping software to fulfill its critical role as a cornerstone of long-term CSE collaboration.

Organizer: David E. Bernholdt
Oak Ridge National Laboratory, USA

Organizer: Michael Heroux
Sandia National Laboratories, USA

Organizer: Daniel S. Katz
University of Illinois at Urbana-Champaign, USA

Organizer: Lois Curfman McInnes
Argonne National Laboratory, USA

1:30-1:50 Potential for Big Data Technologies to Radically Change the Software Engineering of HPC Visualization and Analysis Tools
Mark Miller, Lawrence Livermore National Laboratory, USA

1:55-2:15 A Software Infrastructure for Solving Quantum Physics Problems on Extremely Parallel Systems
Achim Basermann, Jonas Thies and Melven Roehrig-Zoellner, German Aerospace Center (DLR), Germany

2:20-2:40 Role of the Molecular Science Software Institute Toward Sustainable Software
Theresa Windus, Iowa State University, USA; Daniel Crawford, Virginia Tech, USA; Cecilia Clementi, Rice University, USA; Robert Harrison, Brookhaven National Laboratory and Stony Brook University, USA; Teresa Head-Gordon, University of California, Berkeley, USA; Shantenu Jha, Rutgers University, USA; Anna Krylov, University of Southern California, USA; Vijay Pande, Stanford University, USA

2:45-3:05 What We Have Learned About Using Software Engineering Practices in Scientific Software
Jeffrey C. Carver, University of Alabama, USA

continued in next column

Wednesday, March 1

MS172

Reduced Order Modeling Techniques in Large Scale & Data-Driven PDE Problems - Part II of II

1:30 PM-3:10 PM

Room:205

For Part 1 see MS145

A growing number of applications in engineering merge mathematical models built on partial differential equations and complex data (possibly high-dimensional and/or affected by uncertainty) in order to perform tasks such as driving a system to a desired target, ensuring minimal operational risk, identifying unknown or uncertain features or efficiently exploring different scenarios. Data assimilation and uncertainty quantification problems, as well as multiscale and/or multiphysics problems, are currently open challenges for reduced order modeling techniques: whilst making the solution of these many-query, and potentially large- scale, problems computationally tractable, many outstanding theoretical and algorithmic challenges remain. The goal of this minisymposium is to bring together researchers who are active in the aforementioned fields, to present novel and promising methods, and to discuss future trends for research in the field of reduced order modeling.

Organizer: Andrea Manzoni
École Polytechnique Fédérale de Lausanne, Switzerland

Organizer: Matthew J. Zahr
Stanford University, USA

1:30-1:50 Manifold Clustering for Nonlinear Local Reduced Order Structural Models with Contact
Todd Chapman, Stanford University, USA

continued on next page

1:55-2:15 Error Surrogates for Reduced-Order Models Based on Machine Learning Techniques

Stefano Pagani, Politecnico di Milano, Italy; Kevin T. Carlberg, Sandia National Laboratories, USA; Andrea Manzoni, École Polytechnique Fédérale de Lausanne, Switzerland

2:20-2:40 Lagrangian Basis Method for Dimensionality Reduction of Convection Dominated Nonlinear Flows

Rambod Mojgani and Maciej Balajewicz, University of Illinois at Urbana-Champaign, USA

2:45-3:05 Modeling and Predicting Reversals of Earth's Dipole by Low-Dimensional Models

Matthias Morzfeld, University of Arizona, USA; Alexandre Fournier and Gauthier Hulot, Institut de Physique du Globe de Paris, France

Wednesday, March 1

MS173

Novel Numerical Methods for Maxwell's Equations and Magnetohydrodynamics - Part II of II

1:30 PM-3:10 PM

Room:206

For Part 1 see MS146

Maxwell's equations describe how electric and magnetic fields interact. Magnetohydrodynamics (MHD) models the magnetic properties of electrically conducting fluids. Both involve fundamental and important systems of partial differential equations that have wide range of applications such as fusion, astrophysical phenomena, and electromagnetic materials. The main theme of the minisymposium is on the advanced numerical methods for solving these types of models. The focus is on robust temporal and spatial discretizations, efficient nonlinear and linear solvers, and practical implementations for a wide range of applications related to Maxwell's equations and the MHD model.

Organizer: Xiaozhe Hu
Tufts University, USA

Organizer: James H. Adler
Tufts University, USA

1:30-1:50 Mimetic Finite Difference Schemes for Maxwell Equations

Carmen Rodrigo, University of Zaragoza, Spain; James H. Adler, Tufts University, USA; Francisco José Gaspar, University of Zaragoza, Spain; Xiaozhe Hu, Tufts University, USA; Ludmil Zikatanov, Pennsylvania State University, USA

continued in next column

1:55-2:15 Scalable Block Preconditioners for Maxwell's Equations and Continuum Plasma Physics Models

Edward G. Phillips, John Shadid, and Eric C. Cyr, Sandia National Laboratories, USA

2:20-2:40 Parallel Monolithic Multigrid Preconditioners for MHD

Thomas Benson, Lawrence Livermore National Laboratory, USA; Scott Maclachlan, Memorial University, Newfoundland, Canada; James H. Adler, Tufts University, USA; Raymond S. Tuminaro and Eric Cyr, Sandia National Laboratories, USA

2:45-3:05 A Generalized Approach for Scalable N-Body Calculations

Scott High, Michigan State University, USA; Natalie N. Beams, Jonathan B. Freund, and Luke Olson, University of Illinois at Urbana-Champaign, USA

Wednesday, March 1

MS174

Advances in Computational Fractional PDEs - Part II of II

1:30 PM-3:10 PM

Room:209

For Part 1 see MS147

Development of highly efficient and accurate computational methods for fractional PDEs is a challenging area due to the nonlocality of the derivative terms. This requires special treatment of the fractional derivatives while maintain higher order of accuracy. Fractional models are considered heavily to account for anomalous diffusion and dispersion that takes place in many applications. Designing effective schemes based on FD, FEM, and spectral methods, by utilizing special time integrators, and stochastic simulation, create serious challenges for efficient and fast algorithms. The minisymposium will report the recent advances in the computational methods for deterministic and stochastic fractional models. The talks in this minisymposium will present a broad range of tools, methods, venues, problems, and applications.

Organizer: Abdul Khaliq

Middle Tennessee State University, USA

Organizer: Khaled Furati

King Fahd University of Petroleum and Minerals, Saudi Arabia

Organizer: Mohsen Zayernouri

Michigan State University, USA

1:30-1:50 Highly Efficient Methods for Space-Fractional Reaction-Diffusion Systems

Khaled Furati and Mohammad Yousuf, King Fahd University of Petroleum and Minerals, Saudi Arabia; Harish Bhatt, Texas A&M University, USA; Abdul Khaliq, Middle Tennessee State University, USA

1:55-2:15 Fractional-Order Modeling and Simulation of the Human Ear System

Maryam Naghibolhosseini, Michigan State University, USA

2:20-2:40 Well-Balanced Central Fractional Derivatives in Reaction-Diffusion Modeling Applications

Qin Sheng, Baylor University, USA; Haiwei Sun, University of Macau, China; Yufeng Xu, Central South University, China

2:45-3:05 A Second Order Finite Difference Method for Time-Space Fractional Diffusion Equations with Riesz Derivative

Sadia Arshad, COMSATS Institute of Information Technology, Lahore, Pakistan; Jianfei Huang, Qingdao University, China; Yifa Tang, Chinese Academy of Sciences, China

continued in next column

Wednesday, March 1

MS175

Taming the Beast: Broadening the Applicability of Algebraic Multigrid - Part II of II

1:30 PM-2:45 PM

Room:210

For Part 1 see MS148

In theory, everything works in practice. In practice, algebraic multigrid (AMG) can be a sensitive method. For certain classes of problems, AMG has proven to be a fast and scalable solver for large, sparse linear systems. However, AMG can be less robust when extended to more general systems than well-behaved M-matrices. In this minisymposium, theoretical observations are used to motivate practical AMG methods that broaden the applicability of AMG. Convergence theory for AMG is discussed, along with the optimal interpolation operator with respect to two-grid convergence. Practical ways of achieving theoretical convergence and approximating such an operator are presented, with numerical results from a wide class of problems resulting from the discretization of partial differential equations (PDEs). Convergence theory is connected with PDE discretization by considering how to efficiently achieve full-multigrid like behavior, i.e. achieve discretization accuracy, in an AMG algorithm, and methods to reduce communication in the parallel setting are presented. AMG is also extended to linear systems resulting from the study of graph Laplacians for undirected, directed, and signed graphs, and nonlinear system of equations that show up in power grid simulations.

Organizer: Ben Southworth

University of Colorado Boulder, USA

continued on next page

1:30-1:50 Reducing Parallel Communication Costs in Algebraic Multigrid

Amanda Bienz, William D. Gropp, and Luke Olson, University of Illinois at Urbana-Champaign, USA

1:55-2:15 Algebraic Multigrid for Directed Graph Laplacian Systems

Alyson Fox, University of Colorado Boulder, USA; Geoff Sanders, Lawrence Livermore National Laboratory, USA; Thomas Manteuffel, University of Colorado Boulder, USA

2:20-2:40 Nonlinear Algebraic Multigrid for the Power Flow Equations

Colin Ponce and Panayot Vassilevski, Lawrence Livermore National Laboratory, USA; David Bindel, Cornell University, USA

Wednesday, March 1

MS176

Liquid Crystals and Related Models, Computation, and Applications - Part II of II

1:30 PM-3:10 PM

Room:211

For Part 1 see MS149

Liquid crystals are a work-horse technology in industry (e.g. for electronic displays). But there are many other potential technological uses of liquid crystals, such as in material design. In addition, liquid crystal models find use in modeling "active matter" systems. Therefore, new methods are needed to model, analyze, simulate, and control these systems. This minisymposium will deliver a range of talks on modeling/theory, numerical analysis, and applications related to liquid crystals.

Organizer: Shawn W. Walker
Louisiana State University, USA

Organizer: Noel J. Walkington
Carnegie Mellon University, USA

Organizer: Amanda E. Diegel
Louisiana State University, USA

1:30-1:50 Active Liquid Crystals and their Applications to Cell Motility

Qi Wang, University of South Carolina, USA and Beijing Computational Science Research Center, China

1:55-2:15 On Energy Stable Shemes for a Hydrodynamic Q-Tensor Model of Liquid Crystals

Jia Zhao, University of North Carolina at Chapel Hill, USA; Xiaofeng Yang, University of South Carolina, USA; Qi Wang, University of South Carolina, USA and Beijing Computational Science Research Center, China

2:20-2:40 Numerical Approximations to a New Phase Field Model for Two Phase Flows of Complex Fluids

Xiaofeng Yang, University of South Carolina, USA

2:45-3:05 A Direct Proof on the Eigenvalue Preservation for the Beris-Edward System Modeling Liquid Crystals

Xiang Xu, Old Dominion University, USA

Wednesday, March 1

MS177

Innovative Algorithms for Eigenvalue and Singular Value Decomposition - Part II of II

1:30 PM-3:10 PM

Room:212

For Part 1 see MS150

The minisymposium will focuses on the first steps taken on the development of novel software methodologies and algorithm for the next generation of HPC systems. Some scale challenges will be addressed; the goal is to close the "application-architecture peak performance gap" by exploring algorithms and runtime improvements that will enable key science applications to better exploit the architectural features of the extreme-scale systems. The contributed talks will cover new approaches that can overcome the limitations of existing dense/sparse eigensolver libraries on platforms that require fine granularity and memory-aware computational tasks combined with asynchronism in parallel execution.

Organizer: Azzam Haidar
University of Tennessee, USA

1:30-1:50 Efficient Transformation of the General Eigenproblem with Symmetric Banded Matrices to a Banded Standard Eigenproblem

Michael Rippl and Thomas K. Huckle, Technische Universität München, Germany; Bruno Lang, University of Wuppertal, Germany

1:55-2:15 Accelerating the Singular Value Decomposition with a Hybrid Two-Stage Algorithm

Mark Gates and Azzam Haidar, University of Tennessee, USA; Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA

2:20-2:40 Fast Batched SVD on GPUs

Wajih Halim Boukaram, David E. Keyes, and Hatem Ltaief, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; George M Turkiyyah, American University of Beirut, Lebanon

2:45-3:05 Some Notes on Divide-and-Conquer Eigensolvers

Wilfried N. Gansterer, Michael Moldaschl, and Kastor Felsner, University of Vienna, Austria

Wednesday, March 1

MS178

Collocation Methods for High-Dimensional Parameterized Problems in Uncertainty Quantification - Part II of II

1:30 PM-2:45 PM

Room:213

For Part 1 see MS151

Many problems in uncertainty quantification rely on robust and efficient parametric collocation approximations. Collocation methods are attractive because they are simple, non-intrusive, and are flexible enough to exploit structure such as smoothness, sparsity, low-rank manifolds, or low intrinsic-dimensionality. The current challenges that this minisymposium aims to address involve quasi-optimal distributions for approximation, robust quadrature, dimensional scaling, measure adaptivity, and Bayesian inference. This minisymposium bring together researchers from across the applied and computational mathematics community to discuss and collaborate on novel theoretical and computational advances in collocation strategies, and to discuss future directions for research.

Organizer: John D. Jakeman

Sandia National Laboratories, USA

1:30-1:50 Continuous Alternating Least Squares for Regression of Low-Rank Functions

Alex A. Gorodetsky, Massachusetts Institute of Technology, USA; John D. Jakeman, Sandia National Laboratories, USA

1:55-2:15 Low Rank Approximation and Integration of High Dimensional Functions for Quantum Chemistry Applications

Prashant Rai, Khachik Sargsyan, and Habib N. Najm, Sandia National Laboratories, USA; Matthew Hermes and So Hirata, University of Illinois at Urbana-Champaign, USA

2:20-2:40 A New Sampling Method for Alternating Least-Squares Regression

Matthew Reynolds and Alireza Doostan, University of Colorado Boulder, USA

Wednesday, March 1

MS179

Sparse Matrix Ordering Techniques

1:30 PM-3:10 PM

Room:214

In this minisymposium, we are interested in sparse matrix ordering techniques. Computing an an ordering is equivalent to re-ordering vertices in a graph. Many sparse matrix computations rely heavily on matrix ordering strategies. Sparse linear direct solvers try to minimize fill, while iterative solvers try to maximize locality. Solvers using low-rank approximations may also try to reorder the input matrix so as to reduce the ranks of the sub-blocks, leading to lower computational costs. Matrix orderings are thus key to many scientific computations.

Organizer: Mathias Jacquelin

Lawrence Berkeley National Laboratory, USA

Organizer: Esmond G. Ng

Lawrence Berkeley National Laboratory, USA

1:30-1:50 Impact of Blocking Strategies for Sparse Direct Solvers on Top of Generic Runtimes

Gregoire Pichon, *Mathieu Faverge*, and Pierre Ramet, Université de Bordeaux, Inria, LaBRI, France; Jean Roman, Inria, France

1:55-2:15 Refined Ordering in Supernodes to Improve Block Structure and Data Locality

Mathias Jacquelin, Lawrence Berkeley National Laboratory, USA; Barry Peyton, Dalton State College, USA; Esmond G. Ng, Lawrence Berkeley National Laboratory, USA

2:20-2:40 Reducing the Complexity of the Minimum Local Fill Algorithm

Barry Peyton, Dalton State College, USA; Mathias Jacquelin and Esmond G. Ng, Lawrence Berkeley National Laboratory, USA

2:45-3:05 Distributed-Memory Graph Ordering

Ariful Azad, *Aydin Buluc*, Mathias Jacquelin, and Esmond G. Ng, Lawrence Berkeley National Laboratory, USA

Wednesday, March 1

MS180

Invariant Domain and Asymptotic Preserving Techniques for Hyperbolic Systems - Part II of II

1:30 PM-3:10 PM

Room:215

For Part 1 see MS153

Positive density and internal energy are invariant properties for the Euler equations; likewise, positive water height is an invariant property of the shallow water equations. Many first-order methods are known to be invariant-domain preserving, but extending theses techniques to higher-order is non-trivial. The difficulty consists of being invariant, high-order accurate and to satisfy enough entropy inequalities for the approximation to converge to an entropy solution. Invariant-domain preserving are important in applications where being 'in bounds' is essential. The objective of minisymposium is to gather specialists to present the latest developments on invariant-domain preserving methods for the approximation of hyperbolic systems.

Organizer: Jean-Luc Guermond

Texas A &M University, USA

1:30-1:50 High Order Maximum Principle Preserving Semi-Lagrangian Finite Difference Weno Schemes for the Vlasov Equation

Jingmei Qiu, University of Houston, USA

1:55-2:15 Modelling Liquid-Vapor Phase Change with Metastability

Helene Mathis, Université de Nantes, France

2:20-2:40 Low-Dissipation Centred Fluxes for Discontinuous Galerkin Finite Element Methods

Eleuterio F. Toro and Beatrice Saggiorato, University of Trento, Italy; Svetlana Tokareva, University of Zurich, Switzerland

2:45-3:05 Positivity-Preserving Well-Balanced Discontinuous Galerkin Method for Tidal Bores

Yulong Xing, University of California, Riverside, USA

Wednesday, March 1

MS181

Flooding the Cores - Computing Flooding Events on Modern Architectures - Part II of II

1:30 PM-3:10 PM

Room:216

For Part 1 see MS154

Detailed simulation of flooding events, such as storm surges, tsunamis or overland floods, requires substantial computing power. Supercomputing technology today is characterized by an increasing amount of parallelism on all scales. Hence, numerical methods, algorithms and software need to be tuned for data parallelism, multi- and many-core compute nodes (including accelerator technology) and large-scale parallelism. This minisymposium thus focuses on how to literally flood the cores with simulation tasks. We will discuss approaches to reduce time to solution for simulating complex flooding events on supercomputers and architectures characterized by many-core and accelerator technologies, including GPUs and Xeon Phis.

Organizer: Michael Bader
Technische Universität München, Germany

Organizer: Tobias Weinzierl
Durham University, United Kingdom

Organizer: Kyle T. Mandli
Columbia University, USA

1:30-1:50 Many Waves on Many Cores
Dominic E. Charrier and Tobias Weinzierl, Durham University, United Kingdom

1:55-2:15 Modeling the 1976 Teton Dam Failure using GeoClaw
Donna Calhoun, Boise State University, USA; Melody Shih and Kyle T. Mandli, Columbia University, USA

2:20-2:40 Performance and Time to Solution of Dynamically Adaptive Tsunami Simulations
Chaulio Ferreira, Leonhard Rannabauer, and Michael Bader, Technische Universität München, Germany

2:45-3:05 Metaprogramming for Unstructured-Mesh Applications in Ocean Modeling
Harald Koestler and Sebastian Kuckuk, University of Erlangen-Nuernberg, Germany

Wednesday, March 1

MS182

Challenges and Approaches for Enabling Large-Scale Molecular Simulation - Part II of II

1:30 PM-3:10 PM

Room:217

For Part 1 see MS155

Molecular simulation is a powerful technique to investigate chemical/biological processes, and materials properties. Molecular dynamics (MD) simulations are characterized by a force field, involving many parameters to describe the interactions between atoms. Accurately accounting for these interactions constrains the timestep lengths in MD simulations to femtoseconds, while several chemical or biological processes of interest take place in the span of seconds and beyond. Today, state of the art simulations on general purpose computers are way behind this target. While the significantly improved computational power of modern clusters provide an exciting opportunity, important challenges need to be addressed to fully leverage the potential of today's processors and accelerators in MD simulations. First and foremost, parallelism at each level (vector processing, shared memory and distributed memory) must be exploited to obtain the best absolute performance. Novel numerical methods, better integrators and enhanced sampling techniques can complement parallelism to significantly improve the temporal span of MD simulations. Finally, solutions must be portable across different architectures and the large variety of molecular force fields actively used in the community. This minisymposium brings together experts to explore potential solutions across the spectrum of challenges faced by the molecular simulation community.

continued in next column

Organizer: H. Metin Aktulga
Michigan State University, USA

Organizer: William J. Mcdoniel
RWTH Aachen University, Germany

1:30-1:50 Particle-Particle Particle-Mesh (P3M) on Knights Landing Processors
William J. Mcdoniel and Paolo Bientinesi, RWTH Aachen University, Germany; Ahmed E. Ismail, West Virginia University, USA; Markus Höhnerbach and Rodrigo Canales, RWTH Aachen University, Germany

1:55-2:15 Multilevel Summation Method for Efficient Computation of Nonbonded Forces in Molecular Dynamics Simulations
David J. Hardy, University of Illinois at Urbana-Champaign, USA; Robert D. Skeel, Purdue University, USA

2:20-2:40 Towards Autotuning Between OpenMP Schemes for Molecular Dynamics on Intel Xeon Phi
Nikola P. Tchipev, Andrei Costinescu, Steffen Seckler, Philipp Neumann, and Hans-Joachim Bungartz, Technische Universität München, Germany

2:45-3:05 Vectorization of Multi-Body Potentials: Performance and Portability
Paolo Bientinesi and Markus Höhnerbach, RWTH Aachen University, Germany; Ahmed E. Ismail, West Virginia University, USA

Wednesday, March 1

MS183

Understanding Performance Variability Due to Application-Data Center Interaction - Part II of II

1:30 PM-3:10 PM

Room:218

For Part 1 see MS156

System issues and applications' contention for resources can adversely impact system efficiency and application runtimes resulting in large performance variability. Attributing performance issues to specific root causes, and quantifying the impact under production conditions are difficult. Recent advances in platform and application instrumentation, along with data analytics and visualization techniques for high-volume, multi-dimensional data, can provide the basis for such evaluations. This minisymposium brings together experts in these areas to discuss current techniques and progress in detection, understanding, and attribution of system and application performance issues and how such insight is being used to improve application performance and system operations.

Organizer: James Brandt

Sandia National Laboratories, USA

Organizer: Ann Gentile

Sandia National Laboratories, USA

Organizer: Abhinav Bhatele

Lawrence Livermore National Laboratory, USA

Organizer: Todd Gamblin

Lawrence Livermore National Laboratory, USA

1:30-1:50 Detecting and Attributing Application Performance Anomalies to Root Causes

Abhinav Bhatele, Lawrence Livermore National Laboratory, USA; Staci Smith and David K. Lowenthal, University of Arizona, USA; Vanessa Cedeno, Virginia Tech, USA; Todd Gamblin, Lawrence Livermore National Laboratory, USA

continued in next column

1:55-2:15 Resource Management Techniques for Reducing Interference Among Message-Passing Applications

Ana Jokanovic and Jose Carlos Sancho, Barcelona Supercomputing Center, Spain; German Rodriguez, Rockley Photonics, USA

2:20-2:40 Understanding and Avoiding Performance Variability in High Performance Networks

Ryan Grant, Sandia National Laboratories and University of New Mexico, USA; Taylor Groves, University of New Mexico, USA; Kevin Pedretti and Ann Gentile, Sandia National Laboratories, USA; Dorian Arnold, University of New Mexico, USA

2:45-3:05 TOKIO: Using Lightweight Holistic Characterization to Understand, Model, and Improve HPC I/O Performance

Philip Carns, Argonne National Laboratory, USA

Wednesday, March 1

MS184

Advances in Dynamic Graphs: Algorithms, Applications and Challenges - Part II of II

1:30 PM-3:10 PM

Room:219

For Part 1 see MS157

Many interesting phenomena can be modeled as dynamic graphs. For example, in biology, complex interactions of microbes evolve over a period of time; in cybersecurity, malicious activities evolve over a period of time through complex interactions with the system; and in transportation networks, dynamic analysis of traffic is essential for modeling evacuation plans and contingency measures. Several graph algorithms such as dynamic community detection, network alignment, graph matching and edge cover formulations play a vital role in the study of real-world dynamic networks. The goal of this minisymposium is to bring together computational researchers and domain experts exploring dynamic graph models, algorithms, and applications of interest. We propose a two-part minisymposium covering problems from application domains in biology (microbial communities, brain networks), cybersecurity (anomaly detection, control systems), and transportation networks. These talks will be augmented with talks on dynamic graph algorithmic modeling, design and development at scale.

Organizer: Ananth Kalyanaraman

Washington State University, USA

Organizer: Mahantesh Halappanavar

Pacific Northwest National Laboratory, USA

continued on next page

1:30-1:50 Models for Principled Characterization of Dynamic, Spatially Embedded, Multiscale Networks
Danielle Bassett and Richard betzel, University of Pennsylvania, USA

1:55-2:15 Scalable Algorithms for Graph Matching and Edge Cover Computations
Alex Pothen and Arif Khan, Purdue University, USA; Mostofa Patwary and Pradeep Dubey, Intel Labs, USA

2:20-2:40 Massive-Scale Streaming Analytics for Dynamic Graphs
David A. Bader, Georgia Institute of Technology, USA

2:45-3:05 Dynamic Network Analysis: From Inference to Insight
Tanya Y. Berger-Wolf, University of Illinois, Chicago, USA

Wednesday, March 1

MS185

Multi-Fidelity and Multi-Information-Source Methods - Part II of II

1:30 PM-3:10 PM

Room:220

For Part 1 see MS158

Analysis and decision-making processes for complex, multidisciplinary systems often begin with low-fidelity models and progressively incorporate higher fidelity tools. In many cases, however, there is not just a set of computational models clearly ranked in terms of fidelity. Rather, there are multiple models with different types of distortion of the true system. Moreover often the analysis and decision involve other information sources (e.g., expert opinion, experiments). Typically, these different information sources are combined in an ad hoc manner. This minisymposium features research that is developing principled approaches that explicitly integrate the breadth of available information sources.

Organizer: Karen E. Willcox

Massachusetts Institute of Technology, USA

1:30-1:50 Modeling and Identification of Multi-Physics Uncertainties in the Response of Heated Structures
Pengchao Song, X.Q. Wang, and *Marc P. Mignolet*, Arizona State University, USA

1:55-2:15 Sparsity Identification in Non-Gaussian Distributions, with Applications to Multi-Disciplinary Systems
Rebecca Morrison and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

2:20-2:40 Lookahead in Single and Multiple Fidelity Bayesian Optimization
Brendan Tracey, Santa Fe Institute and Massachusetts Institute of Technology, USA; David Wolpert, Santa Fe Institute, USA

2:45-3:05 Multifidelity Moment Estimation in Coupled Multidisciplinary Systems Under Uncertainty
Anirban Chaudhuri and Karen E. Willcox, Massachusetts Institute of Technology, USA

Wednesday, March 1

MS186

Bridging Macrophysics and Microphysics in Kinetic Plasma Models: Computational Perspectives - Part II of II

1:30 PM-3:10 PM

Room:Crystal AF - 1st Fl

For Part 1 see MS159

Including the microscopic physics in macroscopic computer simulations of magnetized plasmas is a very challenging task since mathematical models, e.g., the Vlasov-Maxwell equations, are relatively highly dimensional, strongly non-linear and extremely multiscale. The strong interest on applications as magnetic fusion energy and astrophysical plasmas and the super-computing architectures available nowadays and in the forthcoming future (from peta-scale to exa-scale computers) are driving the development of new robust and efficient computational approaches and models. This minisymposium aims at gathering researchers and experts in multiscale computational modelling of plasma physics problems, innovative numerical techniques and high performance computing for large-scale computer simulations.

Organizer: Gianmarco Manzini

Los Alamos National Laboratory, USA

Organizer: Gian Luca Delzanno

Los Alamos National Laboratory, USA

1:30-1:50 Method of Lines Transpose (molt), An O(N) Implicit Maxwell Solver Coupled with Particle in Cell
Andrew J. Christlieb, Yingda Cheng, and Wei Guo, Michigan State University, USA

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Wednesday, March 1

MS186

Bridging Macrophysics and Microphysics in Kinetic Plasma Models: Computational Perspectives - Part II of II

1:30 PM-3:10 PM

continued

1:55-2:15 Semi-Lagrangian Solution of the Gyrokinetic Vlasov Equation: Latest Developments in the Selalib Code

Yaman Güçlü, Max-Planck-Institut für Plasmaphysik, Germany; Michel Mehrenberger and Laura Mendoza, University of Strasbourg, France; Ahmed Ratnani, Max-Planck-Institut für Plasmaphysik, Germany; Eric Sonnendrücker, Max-Planck-Institut für Plasmaphysik and Technische Universität München, Germany; Edoardo Zoni, Technische Universität München, Germany

2:20-2:40 An Eulerian Discontinuous Galerkin Scheme for the Fully Kinetic Vlasov-Maxwell System

Jason TenBarge and James Juno, University of Maryland, USA; Ammar Hakim, Princeton Plasma Physics Laboratory, USA

2:45-3:05 MHD with Embedded Particle-in-Cell (MHD-EPIC): Capturing Kinetic Effects in Global Simulations

Yuxi Chen and Gabor Toth, University of Michigan, USA; Stefano Markidis and Ivy Bo Peng, KTH Royal Institute of Technology, Sweden

Wednesday, March 1

MS187

Fast Solvers for Large-Scale Inverse Problems in Imaging - Part II of II

1:30 PM-3:10 PM

Room:Crystal CD - 1st Fl

For Part 1 see MS160

We discuss recent advances in algorithms for large-scale inverse problems in the imaging sciences. Due to ill-conditioning, non-convexity, large problem size, infinite-dimensional structure, and the need for adjoint operators, such problems are challenging to solve. Key algorithmic challenges include computational complexity, memory consumption, a vast number unknowns as well as model and data uncertainties. We showcase state-of-the-art techniques in scientific computing to tackle these challenges.

Organizer: Andreas Mang

University of Texas at Austin, USA

Organizer: George Biros

University of Texas at Austin, USA

1:30-1:50 Efficient Solvers for Coupled Imaging Problems

James Herring and Lars Ruthotto, Emory University, USA

1:55-2:15 Arock: An Algorithmic Framework for Asynchronous Parallel Coordinate Updates

Ming Yan, Michigan State University, USA; Zhimin Peng, University of California, Los Angeles, USA; Yangyang Xu, University of Alabama, USA; Wotao Yin, University of California, Los Angeles, USA

2:20-2:40 Scalable Solvers for Joint Inversion with Several Structural Coupling Terms

Benjamin Crestel and Tan Bui-Thanh, University of Texas at Austin, USA; Georg Stadler, Courant Institute of Mathematical Sciences, New York University, USA; Omar Ghattas, University of Texas at Austin, USA

2:45-3:05 Parallel Algorithms for PDE-Constrained Optimization Problems with Hyperbolic Constraints

Andreas Mang, Amir Gholaminejad, and George Biros, University of Texas at Austin, USA

Wednesday, March 1

MS188

Reduced Order Models for Fluids: Achievements and Open Problems - Part II of II

1:30 PM-3:10 PM

Room:301

For Part 1 see MS161

This minisymposium aims at giving a survey of recent developments in the reduced order modeling of fluid flows. Computational modeling, numerical analysis and applications to realistic engineering and geophysical flow problems will be covered in this minisymposium. Both achievements and open problems in the reduced order modeling of fluid flows will be discussed.

Organizer: Jeff Borggaard

Virginia Tech, USA

Organizer: Lizette Zietsman

Virginia Tech, USA

1:30-1:50 Using Derivative Snapshots in ROMs – Error Estimates for Linear Systems, Error Bounds for Nonlinear Systems and Numerical Examples

Tanya Kostova-Vassilevska, Lawrence Livermore National Laboratory, USA

1:55-2:15 Incremental POD Method of Snapshots for Finite Element Fluid Computations

Hiba Fareed, Missouri University of Science and Technology, USA; Jiguang Shen, University of Minnesota, USA; *John Singler* and Yangwen Zhang, Missouri University of Science and Technology, USA

2:20-2:40 Computational Reduction Strategies for Bifurcations and Stability Analysis in Fluid-Dynamics: Applications to Coanda Effect

Giuseppe Pitton, SISSA, International School for Advanced Studies, Trieste, Italy; *Annalisa Quaini*, University of Houston, USA; Gianluigi Rozza, SISSA-ISAS International School for Advanced Studies, Italy

2:45-3:05 Spectral Density of the Koopman Operator: Interpretation and Approximation

Marko Budisic, Clarkson University, USA; Ryan Mohr and Mihai Putinar, University of California, Santa Barbara, USA

Wednesday, March 1

MS189

Model Reduction for Optimal Control Problems: Perspectives from Junior Researchers - Part II of II

1:30 PM-3:10 PM

Room:302

For Part 1 see MS162

Optimization and control of systems governed by partial differential equations usually requires expensive evaluations of the forward problem or the optimality system. In a time-critical application such as control, this is often prohibitive, and model reduction can circumvent that problem. In the proposed session, junior researchers such as Ph.D students and PostDocs will present various approaches to model reduction in the context of control. We will consider nonlinear optimization, high-dimensional parameter spaces and feedback control and a variety of applications.

Organizer: Alessandro Alla

Florida State University, USA

1:30-1:50 Efficient PDE-Constrained Optimization under Uncertainty using Adaptive Model Reduction and Sparse Grids

Matthew J. Zahr, Stanford University, USA; Kevin T. Carlberg and Drew P. Kouri, Sandia National Laboratories, USA

1:55-2:15 Accelerating Newton's Method for Large-Scale Time-Dependent Optimal Control via Reduced-Order Modeling

Caleb C. Magruder and Matthias Heinkenschloss, Rice University, USA

2:20-2:40 Pod-Based Multiobjective Optimal Control by Use of the Reference Point Method

Dennis Beermann, Universität Konstanz, Germany

2:45-3:05 Reduced Order Modelling for Fluid-Structure Interaction and Optimal Control Problems

Francesco Ballarin and Gianluigi Rozza, SISSA-ISAS International School for Advanced Studies, Italy

Wednesday, March 1

MS190

Data-Driven Fractional PDE Modeling, Simulation and Prediction - Part II of II

1:30 PM-3:10 PM

Room:303

For Part 1 see MS163

Fractional partial differential equations (FPDEs) are emerging as a powerful tool for modeling challenging multiscale phenomena including overlapping microscopic and macroscopic scales, anomalous transport, and long range time memory or spatial interactions. Compared to integer-order PDEs, the fractional order of the derivatives in FPDEs may be a function of space and time or even a distribution, opening up great opportunities for modeling and simulation of multiphysics phenomena, e.g. seamless transition from wave propagation to diffusion, or from local to non-local dynamics. In addition, data-driven fractional differential operators may be constructed to fit data from a particular experiment or specific phenomenon, including the effect of uncertainties, in which the fractional orders are determined directly from the data, and introducing nonlinearities leading to more complex operators, with one or more fractional orders, capable to model less typical phenomena (such as, for instance, wave propagation in heterogeneous systems). This minisymposium will address FPDE modeling, simulation and prediction and their applications.

Organizer: Hong Wang

University of South Carolina, USA

Organizer: George Em Karniadakis

Brown University, USA

1:30-1:50 Backward Fractional Advection-Dispersion Equations to Predict Contaminant Source

Yong Zhang, University of Alabama, USA; Mark Meerschaert, Michigan State University, USA; Roseanna Neupauer, University of Colorado Boulder, USA

1:55-2:15 An Iterative Mathematical-Computational Framework for Data-Driven FPDE Modelling and Simulation

Mohsen Zayernouri, Michigan State University, USA

2:20-2:40 Fractional Modeling of Multiphase Flows

Fangying Song, Brown University, USA; Chuanju Xu, Xiamen University, China; George Karnidakis, Brown University, USA

2:45-3:05 Title Not Available at Time of Publication

Zhaopeng Hao, Worcester Polytechnic Institute, USA

continued in next column

Wednesday, March 1

MS191

Recent Advances on Numerical Methods and Applications of Phase-field Methods - Part II of II

1:30 PM-3:10 PM

Room:304

For Part 1 see MS164

Interfacial dynamics in complex fluids presents tremendous challenges to science. From a fluid mechanical viewpoint, the essential physics is the coupling between interfacial movement and the flow of the bulk fluids. Phase field (diffuse-interface) methods start from a multi-scale point of view and treat the interface as a microscopic transition zone of small but finite width. Then a set of governing equations can be derived that are thermodynamically consistent and mathematically well-posed. This principle is very powerful and flexible. It has been applied successfully to describe complicated interfaces in various complex fluids. Well designed numerical methods with the diffuse-interface approach can be highly robust and accurate, as long as the interface is well resolved. Phase field methods are now widely used in many branches of science and engineering, such as the material science, biomedical science, biology, chemical engineering. This minisymposium will bring together numerical analysts and computational scientists working on phase field methods to present their recent advances in algorithm designs and applications of phase field methods. The main purposes of this minisymposium are to review the current status, identify problems and future directions, and to promote phase field methods to a wider scientific and engineering community.

continued in next column

Organizer: Xiaofeng Yang
University of South Carolina, USA

Organizer: Jie Shen
Purdue University, USA

1:30-1:50 An Energy Stable Numerical Scheme for the Cahn-Hilliard-Wilmore and Functionalized Cahn-Hilliard Models

Cheng Wang, University of Massachusetts, Dartmouth, USA

1:55-2:15 Numerical Schemes for Phase Field Model for Moving Contact Line Model

Xiaoping Wang, Hong Kong University of Science and Technology, Hong Kong

2:20-2:40 Decoupled, Energy Stable Scheme for Continuum Hydrodynamics Allen-Cahn and Cahn-Hilliard Phase Field Model

Hui Zhang, Beijing Normal University, China

2:45-3:05 A Diffuse Interface Model for Two-Phase Ferrofluid Flows

Ignacio Tomas, Texas A&M University, USA

Wednesday, March 1

MS192

Efficient Algorithms for Bayesian Inverse Problems Governed by PDE Forward Problems - Part II of II

1:30 PM-3:10 PM

Room:305

For Part 1 see MS165

Inverse problems arise when we seek to determine unknown parameters from observational data and mathematical models that relate the parameters to the data. These problems arise across all areas of science, engineering, medicine, and beyond. Inverse problems are often ill-posed; that is, multiple values of the parameters may be consistent with the data to within the noise. Bayesian inference provides a systematic framework for quantifying the resulting uncertainty in the parameters. However, the Bayesian formulation presents significant challenges. First, the parameter to be inferred is often a spatially correlated field, resulting in a high dimensional parameter space after discretization. Second, the forward model is often computationally expensive to solve, particularly when it takes the form of PDEs. The focus of this minisymposium is on recent advances in algorithms for the Bayesian approach to large-scale PDE constrained inverse problems. Specific emphasis is on methods that address the twin challenges of expensive forward problems and high-dimensional parameter spaces. Recent advances in derivative-informed sampling techniques for Markov Chain Monte Carlo, multilevel and high order Quasi Monte Carlo methods, and dimensionality/data reduction techniques will be presented.

Organizer: Vishwas Hebbur Venkata Subba Rao
Virginia Tech, USA

Organizer: Omar Ghattas
University of Texas at Austin, USA

continued on next page

Organizer: Umberto Villa
University of Texas at Austin, USA

Organizer: Tan Bui-Thanh
University of Texas at Austin, USA

1:30-1:50 Joint Model and Parameter Reduction for Large-Scale Bayesian Inversion
Tiangang Cui, Monash University, Australia; Youssef M. Marzouk and Karen E. Willcox, Massachusetts Institute of Technology, USA

1:55-2:15 On Covariance Operators Derived from Elliptic PDEs
Yair Daon, New York University, USA; Georg Stadler, Courant Institute of Mathematical Sciences, New York University, USA

2:20-2:40 Iterative Updating of Model Error for Bayesian Inversion
Matthew M. Dunlop, University of Warwick, United Kingdom; Andrew Stuart, California Institute of Technology, USA; Erkki Somersalo and Daniela Calvetti, Case Western Reserve University, USA

2:45-3:05 Bayesian Calibration of Inadequate Stochastic PDE Models
Umberto Villa, Todd A. Oliver, Robert D. Moser, and Omar Ghattas, University of Texas at Austin, USA

Wednesday, March 1

MS193

Computational Methods for Illumination Optics - Part II of II

1:30 PM-2:45 PM

Room:221

For Part 1 see MS166

The objective of this minisymposium is to present advanced numerical methods that can be used in the design of illumination devices. Examples are Monge-Ampere solvers to compute freeform surfaces or numerical schemes for Liouville's equation from geometrical optics to calculate photomeric variables at the target of a non-imaging optical system.

Organizer: Jan Ten Thije Boonkkamp
Eindhoven University of Technology, Netherlands

1:30-1:50 Eikonals, Ray Mappings and Nonimaging Optics
Jacob Rubinstein, Technion - Israel Institute of Technology, Israel

1:55-2:15 Active Flux Schemes for Liouville's Equation from Geometrical Optics
Bart van Lith, Eindhoven University of Technology, Netherlands

2:20-2:40 A Least-Squares Method for Optical Design
Nitin Kumar Yadav, Eindhoven University of Technology, Netherlands

Wednesday, March 1

MS194

Inverse Problems and Robust Uncertainty Estimation with Applications in Science and Engineering - Part II of II

1:30 PM-2:45 PM

Room:222

For Part 1 see MS167

In industrial science and engineering, experimentation is often driven by the need for data to make specific decisions, but the data itself generally does not inform the decision-making process. Using models of how the data is captured or generated to extract the required information from the measurements is applied inverse problems. There has been a significant shift in industry to solve inverse problems statistically, in order to robustly quantify uncertainties or assign levels of confidence, not just to the data or calculations from the data, but to the final decisions themselves. This minisymposium collects some of the latest research on applied and industrial inverse problems as well as advanced statistical methods for solving them, with an eye towards how the statistical analysis of data can drive decision making in applied and industrial environments.

Organizer: Aaron B. Luttman
National Security Technologies, LLC, USA

1:30-1:50 Uncertainty Quantification in Reduced Order Modeling
Jared Catenacci and Aaron B. Luttman, National Security Technologies, LLC, USA

1:55-2:15 Improved Probabilistic Principal Component Analysis for Application to Reduced Order Modeling
Indika G. Udagedara, Clarkson University, USA

2:20-2:40 On the Role of Physics for Extrapolating First-Principles Models
Kendra Van Buren, Los Alamos National Laboratory, USA

Wednesday, March 1

CP13

Uncertainty Quantification - Part IV of IV

1:30 PM-3:10 PM

Room:223

For Part 3 see CP11

Chair: Peter Arbenz, ETH Zürich, Switzerland

1:30-1:40 A Dictionary Learning Strategy for Bayesian Inference
Lionel Mathelin, CNRS, France

1:42-1:52 Multilevel Monte Carlo Methods for Eigenvalue Problems
Juliette Unwin, Garth Wells, and Nathan Sime, University of Cambridge, United Kingdom

1:54-2:04 Uncertainty Quantification in High Frequency Electromagnetics Using the Low Rank Tucker Decomposition
Dimitrios Loukrezis, Ulrich Roemer, and Herbert De Gersem, Technische Universität Darmstadt, Germany

2:06-2:16 Mode Reduction Methods for Data Assimilation: Subspace Projection Using Koopman Operators
Humberto C. Godinez and Nick Hengartner, Los Alamos National Laboratory, USA

2:18-2:28 Parallel-In-Time Gradient-Type Method For Optimal Control Problems
Xiaodi Deng and Matthias Heinkenschloss, Rice University, USA

2:30-2:40 Simultaneous Estimation of Material Parameters and Neumann Boundary Conditions in a Linear Elastic Model by PDE-Constrained Optimization
Daniel T. Seidl, Bart G. Van Bloemen Waanders, and Timothy Wildey, Sandia National Laboratories, USA

2:42-2:52 Efficient Multilevel Methods for Optimal Control of Elliptic Equations with Stochastic Coefficients
Sumaya Alzuhairy, Andrei Draganescu, and Bedrich Sousedik, University of Maryland, Baltimore County, USA

2:54-3:04 Reduced Order Models for Symmetric Eigenvalue Problems
Peter Arbenz, ETH Zürich, Switzerland; Zlatko Drmac, University of Zagreb, Croatia

Wednesday, March 1

CP14

Numerical PDEs - Part IV of VI

1:30 PM-3:10 PM

Room:224

For Part 3 see CP12
For Part 5 see CP16

Chair: To Be Determined

1:30-1:40 Space-Time Least-Squares Petrov-Galerkin Nonlinear Model Reduction
Youngsoo Choi and Kevin T. Carlberg, Sandia National Laboratories, USA

1:42-1:52 Fluctuating Hydrodynamic Methods for Manifolds: Applications to Microstructures Within Curved Fluid Interfaces
Paul J. Atzberger, University of California, Santa Barbara, USA

1:54-2:04 Curvature-Augmented Numerical Methods for Interfaces and Surfaces
Chris Vogl, University of Washington, USA

2:06-2:16 Algebraic Analysis and Numerical Illustration on Artificial Odd-Even Grid Oscillation and Its Presence in Domain Decomposition Computation
Hansong Tang, City University of New York, USA; Wenbin Dong, City College of CUNY, USA

2:18-2:28 Accelerating Multiscale Coupling Methods in Heterogeneous Adjacent Multidomains with Shear Flow
Xiaocheng Shang and George E. Karniadakis, Brown University, USA

2:30-2:40 A Robust Discontinuous Galerkin Scheme for Ten-Moment Gaussian Closure Equations
Asha K. Meena, Indian Institute of Technology, Delhi, India; Praveen Chandrashekar, TIFR Centre, Bangalore, India; Harish Kumar, Indian Institute of Technology, Delhi, India

2:42-2:52 Solution of PDEs for Photobleaching Kinetics Using Krylov Subspace Spectral Methods
Somayyeh Sheikholeslami and James V. Lambers, University of Southern Mississippi, USA

2:54-3:04 Patient-Specific 3D Reconstruction of Bioresorbable and Metallic Stent: A Critical Step for CFD Analysis of Hemodynamics in Stented Coronary Artery
Boyi Yang, Emory University, USA

Wednesday, March 1

Poster Blitz & Coffee Break

3:10 PM-4:30 PM

Room:Ballroom D - 2nd Fl

PP4

General Posters

4:30 PM-6:30 PM

Room:Galleria

Decay Bounds for Functions of Structured Non-Hermitian Matrices
Stefano Pozza and Valeria Simoncini, Universita' di Bologna, Italy

A Structure Preserving Lanczos Algorithm for Computing the Optical Absorption Spectrum
Meiyue Shao, Lawrence Berkeley National Laboratory, USA; Felipe H. Da Jornada, University of California, Berkeley, USA; Lin Lin, University of California, Berkeley and Lawrence Berkeley National Laboratory, USA; Chao Yang, Lawrence Berkeley National Laboratory, USA; Jack Deslippe, National Energy Research Scientific Computing Center, USA; Steven Louie, University of California, Berkeley, USA

New Rigorous Error Bound For Reduced Basis Approximations
Mladjan Radic and Stefan Hain, Ph.D Student

Numerical Simulation of Poroelastic Wave Equation with Discontinuous Galerkin Using Upwind and Modified Penalty Flux
Khemraj Shukla, Oklahoma State University, USA; Jan S. Hesthaven, École Polytechnique Fédérale de Lausanne, Switzerland; Priyank Jaiswal, Oklahoma State University, USA

Towards the Ultimate Finite Element Method for the Stokes Equations
Hannah M. Morgan and Ridgway Scott, University of Chicago, USA

Low Dispersion Mimetic Discretizations of Maxwell's Equations in Media with Linear Constitutive Laws
Duncan A. McGregor, Sandia National Laboratories, USA

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On the Singular Values Decay of Solutions to a Class of Generalized Sylvester Equations and Efficient Krylov Methods

Davide Palitta, Università di Bologna, Italy; Elias Jarlebring, Giampaolo Mele, and Emil Ringh, KTH Royal Institute of Technology, Sweden

New Second-Order Time Schemes for Optimal Control of Time-Dependent PDEs

Jun Liu, Jackson State University, USA

A Weak Galerkin (WG) Method for Maxwell's Equations in the Time Domain

Sidney R. Shields and Jichun Li, University of Nevada, Las Vegas, USA; Eric Machorro, National Security Technologies, LLC, USA

Adaptive Smoothed Aggregation Episode II: Return of the Bad Guys

Ben Southworth, Steve McCormick, John Ruge, and Tristan Konolidge, University of Colorado Boulder, USA

Advances in Nonlinear Solvers for Coupled Systems

Daniil Svyatskiy, Los Alamos National Laboratory, USA

1D Diffusion with Fractional Laplacian: Regularity and Numerical Methods

Zhongqiang Zhang, Worcester Polytechnic Institute, USA

Numerical Computing with Functions in Polar and Spherical Geometries

Heather D. Wilber and Grady B. Wright, Boise State University, USA; Alex Townsend, Cornell University, USA

An Ale-Level-Set Method for Moving Boundary Problems

Jiaqi Zhang and Pengtao Yue, Virginia Tech, USA

A Stable Added-Mass Partitioned (AMP) Algorithm for Elastic Solids and Incompressible Flows

Daniel A. Serino, Jeffrey W. Banks, William Henshaw, and Donald W. Schwendeman, Rensselaer Polytechnic Institute, USA

Multiscale Energy-Conserving Finite Elements for Atmospheric Flows

Andrea Natale, and Colin J. Cotter, Imperial College, United Kingdom

continued in next column

Quantized Tensor Train and Uniformization Approach for Stochastic Chemical Kinetics

Huy D. Vo and Roger Sidje, University of Alabama, USA

Computing of the Effective Coefficients via Multiscale Discontinuous Galerkin Method

Stanislav Polishchuk, Novosibirsk State Technical University, Russia

Corrugated Coaxial Cable Modeling with a Nodal Discontinuous Galerkin (NDG) Method

Sidney R. Shields and Jichun Li, University of Nevada, Las Vegas, USA; Eric Machorro and Jerome Blair, National Security Technologies, LLC, USA

Numerical Approximations to Katz Centrality

Eisha Nathan, Georgia Institute of Technology, USA; Geoff Sanders and Van Henson, Lawrence Livermore National Laboratory, USA

N Bugs on a Surface

David J. Miller and Bryan D. Quaife, Florida State University, USA

Advancements in Simulation-Based Optimal Experimental Design

Michael Pilosov, University of Colorado, Denver, USA

Fast Algorithms and Computational Software for Obtaining Low Rank Matrix Decompositions

Sergey Voronin, Tufts University, USA; N. Benjamin Erichson, University of St. Andrews, United Kingdom

Mesoscopic and High Performance Modeling of Biomimetic Polymers

Yu-Hang Tang, Zhen Li, and George E. Karniadakis, Brown University, USA

A New 4-Point C^2 Non-Stationary Subdivision Scheme for Computer Geometric Design

Muhammad Younis, University of the Punjab, Lahore, Pakistan

continued in next column

A Semismooth Newton Method for the Solution of a Thermomechanically Coupled Stokes Ice Sheet Model

Hongyu Zhu, University of Texas at Austin, USA; Tobin Isaac, University of Chicago, USA; Georg Stadler, Courant Institute of Mathematical Sciences, New York University, USA; Noemi Petra, University of California, Merced, USA; Thomas Hughes and Omar Ghattas, University of Texas at Austin, USA

Implicit Mesh Discontinuous Galerkin Methods and Interfacial Gauge Methods for High-Order Accurate Interface Dynamics, with Applications to Surface Tension Dynamics, Rigid Body Fluid-Structure Interaction, and Free Surface Flow

Robert Saye, Lawrence Berkeley National Laboratory, USA

Reducing Communication in Distributed Asynchronous Iterative Methods

Jordi Wolfson-Pou, Georgia Institute of Technology, USA

Decentralized Framework for Sensor-Driven Optimization in Power Systems

Paritosh P. Ramanan, Murat Yildirim, Edmond Chow, and Nagi Gebraeel, Georgia Institute of Technology, USA

LOBPCG Method in Exact Diagonalization for Hubbard Model: Performance of Communication Avoiding Neumann Expansion Preconditioner

Susumu Yamada, Japan Atomic Energy Agency, Japan; Toshiyuki Imamura, RIKEN Advanced Institute for Computational Science, Japan; Masahiko Machida, Japan Atomic Energy Agency, Japan

Containers for Scientific Computing: From Laptop to HPC

C N. Richardson and Garth Wells, University of Cambridge, United Kingdom; Jack Hale, University of Luxembourg, Luxembourg

Graph Sparsification Approach for Updating Dynamic Networks on Shared Memory Systems

Sriram Srinivasan, University of Nebraska, Omaha, USA

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Wednesday, March 1

PP4

General Posters

4:30 PM-6:30 PM

continued

Efficient and General Parallel Solver for Boundary Integral Equations

Matthew J. Morse, Abtin Rahimian, and Denis Zorin, Courant Institute of Mathematical Sciences, New York University, USA

A Scalable Linear Solver Based on the FSAI Preconditioner

Victor A. Paludetto Magri, Andrea Franceschini, Carlo Janna, and Massimiliano Ferronato, University of Padova, Italy

Fast Dynamic Load Balancing Tools for Extreme Scale Systems

Cameron Smith and Mark S. Shephard, Rensselaer Polytechnic Institute, USA

Design of a Parallel AMR Infrastructure for Multi-Accelerator Computing

Jaber J. Hasbestan and Inanc Senocak, Boise State University, USA

The Effect of Memory Layout on Batched BLAS Routines

Mawussi Zounon, University of Manchester, United Kingdom; Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA; Nicholas J. Higham, Sven Hammarling, Samuel Relton, and Pedro Valero-Lara, University of Manchester, United Kingdom

Generating Long-Term Wind Scenarios Conditioned on Sequential Forecasts

Kyle Perline, Cornell University, USA; Christine Shoemaker, National University of Singapore, Singapore

A Stochastic Permeability Model for Reduced Order Simulation and Representative Volume Element Prediction

Charles Talbot, Lawrence Livermore National Laboratory and University of North Carolina at Chapel Hill, USA

continued in next column

On Applying Effective Parallelization of Nonlinear Programming to Topology Optimization

Geoffrey M. Oxberry, Mark L. Stowell, Ryan Fellini, Daniel White, and Cosmin G. Petra, Lawrence Livermore National Laboratory, USA

Markov Chain Monte Carlo Optimization for Fitting Excitable Cells Current-Voltage Relations to Voltage Clamp Data

Joseph Mckenna, Florida State University, USA

An Adjoint Capable Solver for the Stefan Problem

Tom O'Leary-Roseberry, Omar Ghattas, Umberto Villa, and Patrick Heimbach, University of Texas at Austin, USA

Coins Classification Using Image Processing and Linear Vector Quantization

Leandro R. Mattioli, Universidade Federal de Uberlandia, Brazil

Stochastic Analysis of Turbulent Mix

Pooja Rao, Stony Brook University, USA; Jeremy A. Melvin, Institute for Computational Engineering and Sciences, USA; Hyunkyung Lim, Stony Brook University, USA; James Glimm, State University of New York, Stony Brook, USA; David Sharp, Los Alamos National Laboratory, USA

Improving RANS Predictive Capability Based on Machine Learning

Jianxun Wang, Jinlong Wu, and Heng Xiao, Virginia Tech, USA

Simulation of Coastal Flows and Waves by Integration of Geophysical Fluid Dynamics and Fully 3D Fluid Dynamics Models

Hansong Tang, City University of New York, USA

Computational Methods to Study the Pattern Formation in Tissues

Xueping Zhao and Qi Wang, University of South Carolina, USA

Modeling the Mitigation of Zika and Chikungunya by Infecting Mosquitoes with Wolbachia Bacteria

Zhuolin Qu, Tulane University, USA; Ling Xue, Harbin Engineering University, China; James Hyman, Tulane University, USA

continued in next column

Apollo: An Unstructured Framework for Multi-Fluid Plasma Modeling

Eder M. Sousa, ERC Inc. and Air Force Research Laboratory , USA

Interior Penalties for Summation-by-Parts Discretizations of Linear Second-Order Differential Equations

Jianfeng Yan, Jared Crean, and Jason E. Hicken, Rensselaer Polytechnic Institute, USA

An Assembly-Free Heterogeneous Computing Method for Simulation of Heat Conduction in Heterogeneous Materials

Andrew Loeb and Chris Earls, Cornell University, USA

A Two Level Preconditioner for Helmholtz Equation in High Frequency Regime

Premkumar Panneerchelvam and Laxminarayan Raja, University of Texas at Austin, USA

Moving Objects Through Phase Change Material - a Hybrid Modeling Approach

Kai Schüller and Julia Kowalski, RWTH Aachen University, Germany

A Plasma-Vacuum Interface Tracking Algorithm for Fully-Implicit Magnetohydrodynamic Simulations

Vivek Subramaniam and Laxminarayan Raja, University of Texas at Austin, USA

A Single-Phase Slightly Compressible Flow and Multicomponent Transport Model in Porous Media at Laboratory Scale

Eduardo Linares-Pérez and Mario Noyola-Rodriguez, Universidad Nacional Autónoma de México, Mexico; Martin A. Diaz-Viera, Instituto Mexicano del Petróleo, México

A Finite Element Discrete Fracture Model to Simulate Fluid Flow Through Fractured Porous Media

Carlos Romano-Pérez, National Autonomous University of Mexico, Mexico; Martin Díaz-Viera, Mexican Petroleum Institute, Mexico

Representation of Discrepancies Between Stress Tensors and Its Application in Data-Driven Turbulence Modeling

Jinlong Wu, Jianxun Wang, and Heng Xiao, Virginia Tech, USA

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Adaptive Sparse Grid Stochastic Collocation for Random Ordinary Differential Equations

Friedrich Menhorn and Tobias Neckel, Technische Universität München, Germany

Adaptive Sparse Grids Interpolation Techniques for Multilevel Stochastic Collocation in Fluid-Structure Interaction Problems

Paul Cristian Sarbu, Ionut-Gabriel Farcas, Benjamin Uekermann, Tobias Neckel, and Hans-Joachim Bungartz, Technische Universität München, Germany

Dynamical Polynomial Chaos Expansions with Applications to Long Time Evolution of SDEs and SPDEs

H. Cagan Ozen and Guillaume Bal, Columbia University, USA

Balanced Iterative Solvers for Linear Systems Arising from Fem Approximation of Pdes with Random Data

Pranjal Pranjal and David Silvester, University of Manchester, United Kingdom

High-Dimensional Function Interpolation with Gradient-Enhanced Weighted ℓ^1 Minimization

Yi Sui and Ben Adcock, Simon Fraser University, Canada

Estimating the Uncertainty of Imprecise Computer Models Using Optimization Methods

Lee R. Redfearn, Clemson University, USA

Neural Networks As Reduced Models for Physical Systems and Inverse Problems

Bassel Saleh, Umberto Villa, and Omar Ghattas, University of Texas at Austin, USA

Model Discrepancy for Simulating Complex Physical Systems: From Data Assimilation to Machine Learning

Heng Xiao, Jinlong Wu, and Jianxun Wang, Virginia Tech, USA

Wednesday, March 1

PP5

General Posters

4:30 PM-6:30 PM

Room:Galleria

Improving Ab Initio Gene Prediction in Prokaryotic Genomes

Karl Gemayel, Shiyuyun Tang, Alexandre Lomsadze, and Mark Borodovsky, Georgia Institute of Technology, USA

Ridge Approximation Using Variable Projection

Jeffrey M. Hokanson and Paul Constantine, Colorado School of Mines, USA

Simulation of Capacitively Coupled Plasmas using a High Performance Parallelized Particle-in-Cell Simulation

Young Hyun Jo, Chang-Ho Kim, Yoon Ho Lee, Geon Woo Park, Jung Yeol Lee, and Hae June Lee, Pusan National Univeristy, South Korea

A Tunably-Accurate Spectral Method with Linear Complexity for Multi-Term Fractional Differential Equations on the Half Line

Anna Lischke and George E. Karniadakis, Brown University, USA; Mohsen Zayernouri, Michigan State University, USA

Likelihood Approximation with Hierarchical Matrices for Large Spatial Datasets}

Alexander Litvinenko, Ying Sun, Marc Genton, and David E. Keyes, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Evaluation of An Improved Numerical Technique for Solving the Hypersonic Boundary Layer/Shockwave Interaction Problem

Julio C. Mendez, David Dodoo-Amoo, and Frederick Ferguson, North Carolina A&T State University, USA

continued in next column

Experiences, Optimizations, and Future Directions with Petsc on the 2nd Generation ("Knights Landing") Intel Xeon Phi Processor

Richard T. Mills, Oak Ridge National Laboratory, USA; Mark Adams, Columbia University, USA; Jed Brown, Argonne National Laboratory and University of Colorado Boulder, USA; Maurice Fabien, Rice University, USA; Tobin Isaac, University of Chicago, USA; Matthew Knepley, Rice University, USA; Karl Rupp, Freelance Computational Scientist, Austria; Barry F. Smith, Argonne National Laboratory, USA

On An Inverse Diffusion Coefficient Problem Arising in Geochronology

Sedar Ngoma and Dmitry Glotov, Auburn University, USA; A. J. Meir, Southern Methodist University, USA; WILLIS E. Hames, Auburn University, USA

An Effect of Turbulence on Zonal Jet Flows in Forced 2D and Quasi-Geostrophic Shallow Water Models on a Beta Plane

Kiori Obuse, Okayama University, Japan; Shin-Ichi Takehiro and Michio Yamda, Kyoto University, Japan

A Computational Model for Sound Source Recognition

Chathurangi H. Pathiravasan and Dinuka Gallaba, Southern Illinois University, Carbondale, USA

Applicability Analysis of Validation Evidence for Biomedical Computational Models

Pras Pathmanathan, Richard Gray, Leonardo Angelone, and Tina Morrison, U.S. Food and Drug Administration, USA

Kronecker Product Preconditioners for Very High Order Discontinuous Galerkin Methods

Will Pazner, Brown University, USA; Per-Olof Persson, University of California, Berkeley, USA

Uncertainties in An Inverse Source Problem for PDE-Constrained Optimization with Inequality Constraints

Widodo Samyono, Columbia University, USA

continued on next page

Wednesday, March 1

PP5

General Posters

4:30 PM-6:30 PM

Room:Galleria

continued

Optimizing and Vectorizing Rank Reduction Techniques in Quantum Chemistry
Matthew C. Schieber, Daniel Smith, and David Sherrill, Georgia Institute of Technology, USA

Nodal Integral Method for Complex Geometries Using Higher Order Elements
Rishabh P. Sharma and Neeraj Kumar, Thapar University, India

A Particle-Based Numerical Method for Solving Vlasov Models in Plasma Simulations
Boqian Shen and James A. Rossmanith, Iowa State University, USA

Positivity-Preserving High Order Discontinuous Galerkin Schemes for Compressible Navier-Stokes
Xiangxiong Zhang, Purdue University, USA

Conservative Exponential Integrators for Nonlinear Conservation Laws
Chad Sockwell, Florida State University, USA

Computation of Electromagnetic Fields Due to Dipoles in Two and Three Layered Media in R^3
Kennedy Udechukwu and Min Hyung Cho, University of Massachusetts, Lowell, USA

Evaluating Production Engineering Application Performance on the Intel Knights Landing Many Core Processor
Simon D. Hammond, *Courtenay T. Vaughan*, Dennis Dinge, Paul Lin, Robert Benner, Christian Trott, Doug Pase, Jeanine Cook, and Robert J. Hoekstra, Sandia National Laboratories, USA

Numerical Interface Treatment for Wave Propagation Problems
Siyang Wang, Uppsala University, Sweden

continued in next column

Sharp Convergence Rates of Numerical Solutions of Stochastic Fractional Equations Driven by White Noise
Max Gunzburger, Florida State University, USA; Buyang Li, Hong Kong Polytechnic University, China; *Jilu Wang*, Florida State University, USA

Analysis of a Preconditioner for Matrices with Block Low-Rank Structure
Xin Xing and Edmond Chow, Georgia Institute of Technology, USA

Application of Optimal Transport and the Quadratic Wasserstein Metric to Full-Waveform Inversion
Yunan Yang and Bjorn Engquist, University of Texas at Austin, USA; Junzhe Sun, ExxonMobil Upstream Research Company, USA; Brittany Froese, New Jersey Institute of Technology, USA

Positivity-Preserving Limiters for the Piecewise-P_N Equations
Minwoo Shin and James A. Rossmanith, Iowa State University, USA

Wednesday, March 1

PP107

Minisymposterium: Broader Engagement Program

4:30 PM-6:30 PM

Room:Galleria

Mary Ann E. Leung, Sustainable Horizons Institute, USA

Wednesday, March 1

PP108

Minisymposterium: Software Productivity and Sustainability for CSE and Data Science

4:30 PM-6:30 PM

Room:Galleria

David E. Bernholdt, Oak Ridge National Laboratory, USA

Michael Heroux, Sandia National Laboratories, USA

Daniel S. Katz, University of Illinois at Urbana-Champaign, USA

Anders Logg, Chalmers University of Technology, Sweden

Lois Curfman McInnes, Argonne National Laboratory, USA

Software is the key crosscutting technology that connects advances in mathematics, computer science, and domain-specific science and engineering to achieve robust simulations and analysis for predictive science, engineering, and other research fields. While software is becoming more complex due to multiphysics and multiscale modeling, the coupling of data analytics, and disruptive changes in computer hardware (due to increases in typical system scale and heterogeneity, including GPUs and additional alternative architectures), software itself has not traditionally received focused attention in the CSE community or been rewarded by that community. The speakers in this minisymposterium will discuss work that addresses growing technical and social challenges in software productivity, quality, and sustainability, and thereby is helping software to fulfill its critical role as a cornerstone of long-term CSE collaboration.

continued in next column

Minisymposterium: Sustainable Productivity in the Fenics Development Team

Martin Alnæs, Simula Research Laboratory, Norway; Jan Blechta, Charles University in Prague, Czech Republic; Jack Hale, University of Luxembourg, Luxembourg; Anders Logg, Chalmers University of Technology, Sweden; C N. Richardson, University of Cambridge, United Kingdom; Johannes Ring, Simula Research Laboratory, Norway; Garth Wells, University of Cambridge, United Kingdom

Minisymposterium: A Sustainable Software Architecture for Scalable Nonlinear Boundary Element Method Simulations

Matthew G. Knepley, Rice University, USA; *Jaydeep P. Bardhan*, Northeastern University, USA

Minisymposterium: The Application of Tribits to the Development and Integration Processes of Larger Componentized Multi-Organization Scientific and Engineering Software Projects

Roscoe A. Bartlett, Sandia National Laboratories, USA

Minisymposterium: Improving Software Productivity of Uintah Through Task-Based Architectures, Performance Portability Libraries and Modern C++ Features

Martin Berzins and *Alan Humphrey*, University of Utah, USA; Dan Sunderland, Sandia National Laboratories, USA; Brad Peterson, University of Utah, USA

Minisymposterium: Doecode: The New Department of Energy Software Center

Jay Billings, Oak Ridge National Laboratory, USA; Mark Martin, DOE Office of Scientific and Technical Information, USA

Minisymposterium: PEACHPY.IO, a Web App for Performance Tuning

Marat Dukhan and Richard Vuduc, Georgia Institute of Technology, USA

Minisymposterium: External Code Review of PFLOTRAN: Lessons Learned

Glenn Hammond, Sandia National Laboratories, USA

continued in next column

Minisymposterium: Regression and Performance Testing and Continuous Integration for Scientific Codes

Timo Heister, Clemson University, USA

Minisymposterium: {CSE} Complete: R & D for Productivity Improvement

Michael Heroux, Sandia National Laboratories, USA; Lois Curfman McInnes, Argonne National Laboratory, USA; David E. Bernholdt, Oak Ridge National Laboratory, USA; David Moulton, Los Alamos National Laboratory, USA

Minisymposterium: CSE Software Maintenance and Automation: Beyond Testing

Dan A. Ibanez, Rensselaer Polytechnic Institute, USA

Minisymposterium: The Impact of Structured AMR Representation on Software Design

Tobin Issac, University of Chicago, USA; Matthew Knepley, Rice University, USA

Minisymposterium: SlabGenerator: Improving Productivity for Subduction Modeling

Margarete A. Jadamec, University of Houston, USA; Matthew Knepley, Rice University, USA

Minisymposterium: HPC Software Productivity Based on High-Level Abstraction in FEniCS

Johan Jansson, *Johan Hoffman*, and Niclas Jansson, KTH Royal Institute of Technology, Sweden

Minisymposterium: System Testing for PDE Frameworks - Tools and Experiences

Dominic Kempf, Universität Heidelberg, Germany; Timo Koch and Bernd Flemisch, Universität Stuttgart, Germany; Peter Bastian, Universität Heidelberg, Germany

continued in next column

continued on next page

Wednesday, March 1

PP108

Minisymposterium: Software Productivity and Sustainability for CSE and Data Science

4:30 PM-6:30 PM

continued

Minisymposterium: Devito: Towards An Efficient and Sustainable Finite Difference DSL

Michael Lange, Imperial College London, United Kingdom; Navjot Kukreja, SENAI CIMATEC, Brazil; Mathias Louboutin, University of British Columbia, Canada; Fabio Luporini, Imperial College London, United Kingdom; Felippe Vieira, SENAI CIMATEC, Brazil; Vincenzo Pandolfo, Imperial College London, United Kingdom; Paulius Velesko, University of Oklahoma, USA; Paulius Kazakas, University of York, United Kingdom; Gerard J. Gorman, Imperial College London, United Kingdom

Minisymposterium: Lessons Learned from Integrating Scientific Libraries Within a Plugin-Based Architecture

Vijay S. Mahadevan, Argonne National Laboratory, USA; Mark Miller, Lawrence Livermore National Laboratory, USA; Iulian Grindeanu, Argonne National Laboratory, USA

Minisymposterium: xSDK: Working toward a Community CSE Software Ecosystem

Lois Curfman McInnes, Argonne National Laboratory, USA; Michael Heroux and Roscoe A. Bartlett, Sandia National Laboratories, USA; Mark Berrill, Oak Ridge National Laboratory, USA; Jeffrey N. Johnson, Lawrence Berkeley National Laboratory, USA; Alicia Klinvex, Sandia National Laboratories, USA; X. Sherry Li, Lawrence Berkeley National Laboratory, USA; J. David Moulton, Los Alamos National Laboratory, USA; Daniel Osei-Kuffuor, Lawrence Livermore National Laboratory, USA; Jason Sarich and Barry F. Smith, Argonne National Laboratory, USA; James Willenbring, Sandia National Laboratories, USA; Ulrike Yang, Lawrence Livermore National Laboratory, USA

continued in next column

Minisymposterium: Sirepo: An Open Source Platform for Portable Reproducible Simulations

Robert Nagler and David Bruhwiler, RadiasSoft LLC, USA; Paul Moeller, Bivio Software, Inc., USA

Minisymposterium: Jupyter Notebooks Facilitating Productivity, Sustainability, and Accessibility of Data Science

Min Ragan-Kelley, Simula Research Laboratory, Norway; Jupyter Development Team, Project Jupyter

Minisymposterium: Practical Approaches to Improve Program Understanding and Software Productivity of Scientific Code

Dali Wang, Oak Ridge National Laboratory, USA; Yu Pei, University of Tennessee, USA; Youngsung Kim, National Center for Atmospheric Research, USA; Oscar Hernandez and David E. Bernholdt, Oak Ridge National Laboratory, USA

Minisymposterium:Maximizing Usability and Performance in Numerical Software Packages

Kanika Sood and Boyana Norris, University of Oregon, USA; Elizabeth Jessup and Pate Motter, University of Colorado, USA

Minisymposterium: Software Productivity Strategies for the Sundials Suite of Time Integrators and Nonlinear Solvers

Carol S. Woodward, Lawrence Livermore National Laboratory, USA; Daniel R. Reynolds, Southern Methodist University, USA; L. Eddy Banks, Lawrence Berkeley National Laboratory, USA; David J. Gardner and Slaven Peles, Lawrence Livermore National Laboratory, USA; Alan Hindmarsh, Lawrence Berkeley National Laboratory, USA

Minisymposterium: Developing Fast Code Through High-Level Annotations

Luke Olson, Bill Gropp, Dan Bodony, Jon Freund, Thiago Teixeira, Tarun Prabhu, Carl Evans, Sam White, Simon Garcia, Cory Mikida, Michael Anderson, Matthew Smith, and John Larson, University of Illinois at Urbana-Champaign, USA

Minisymposterium: GraphFlow: Workflow-Based Big Data Processing

Sara Riazi and Boyana Norris, University of Oregon, USA

Minisymposterium: Numfocus Sustainability Project

Andy R. Terrel, NumFOCUS, USA; *Tracy K. Teal*, Data Carpentry, USA

continued in next column

Minisymposterium: Software Citation Principles for Credit and Reuse

Kyle E. Niemeyer, Oregon State University, USA; Arfon Smith, GitHub, Inc., USA; Daniel S. Katz, University of Illinois at Urbana-Champaign, USA

Minisymposterium: World SpatioTemporal Analytics and Mapping Project (WSTAMP): Cloud Implementation of Open Source Algorithms and Data Stores for Sustainable, Scalable Analysis of Space-Time Data

Robert N. Stewart, Aaron Myers, David Axley, Alex Sorokine, and Jesse Piburn, Oak Ridge National Laboratory, USA

Minisymposterium: The Journal of Open Source Software

Arfon Smith, GitHub, Inc., USA; Lorena Barba, George Washington University, USA; George Githinji, Wellcome Trust, United Kingdom; Melissa Gymrek, University of California, San Diego, USA; Kathryn Huff and Daniel S. Katz, University of Illinois at Urbana-Champaign, USA; Christopher Madan, Boston College, USA; Abigail Cabunoc Mayes, Mozilla Science Laboratory, USA; Kevin Moerman, Massachusetts Institute of Technology, USA; *Kyle E. Niemeyer*, Oregon State University, USA; Pjotr Prins, University of Tennessee, USA; Karthik Ram, University of California, Berkeley, USA; Tracy K. Teal, Data Carpentry, USA; Jake Vanderplas, University of Washington, USA

Minisymposterium: Accelerating Application Software Development Through Software Productivity and Sustainability Plans (PSPs)

David Moulton, Los Alamos National Laboratory, USA; Jeff Johnson, Lawrence Berkeley National Laboratory, USA; Ethan T. Coon, Los Alamos National Laboratory, USA; Carl Steefel and Sergi Molins, Lawrence Berkeley National Laboratory, USA; Glenn Hammond, Sandia National Laboratories, USA; Reed M. Maxwell, Colorado School of Mines, USA; Carol S. Woodward, Lawrence Livermore National Laboratory, USA; Laura Condon, Syracuse University, USA

Minisymposterium: Managing the Scientific Software Ecosystem with Spack

Todd Gamblin, Lawrence Livermore National Laboratory, USA

Thursday, March 2

Registration

7:45 AM-5:00 PM

Room:Foyer - 1st Fl

Announcements

8:10 AM-8:15 AM

Room:Grand Ballroom - 2nd Fl

Thursday, March 2

IP7

Productive and Sustainable: More Effective Computational Science and Engineering

8:15 AM-9:00 AM

Room:Grand Ballroom - 2nd Fl

Chair: Ulrike M. Yang, Lawrence Livermore National Laboratory, USA

Computational Science and Engineering (CSE) is effective to the extent it contributes to overall scientific and engineering pursuits. Its contributions are most tangible when delivering concrete scientific and engineering results via modeling, simulation and analysis. At the same time, delivery of CSE results is impacted by how we develop and support the ecosystem that produced these results, including, in particular, software and people. While delivering results is the ultimate goal of our CSE efforts, the shortest path to results is often not the most productive and sustainable. In this presentation we discuss elements that impact the effectiveness of CSE efforts, beyond just the direct activities to produce results. We discuss how processes, tools and a holistic view of efforts can lead to more effective CSE. We also discuss the importance of human factors in CSE activities, highlighting ways we can provide natural incentives toward more effective CSE.

Michael Heroux

Sandia National Laboratories, USA

CSE Prize Award Ceremony

9:00 AM-9:30 AM

Room:Grand Ballroom - 2nd Fl

Coffee Break

9:30 AM-10:00 AM

Room:Foyer - 2nd Fl

Thursday, March 2

MT7

Interactive CSE with IPython and Jupyter- Part I

10:00 AM-11:40 AM

Room:Ballroom C - 2nd Fl

For Part 2 see MT8

Chair: Min Ragan-Kelley, Simula Research Laboratory, Norway

IPython and Jupyter provide tools for interactive computing that are widely used in science and education, and can benefit any CSE instructor, student, or researcher. We will show how to use IPython to improve your interactive explorations in Python, and how Jupyter notebooks enable interactive exploration, teaching, learning, and reproducibility, in Python as well as other languages such as MatLab, Julia, and R. The first part of the tutorial will focus on using IPython to get the most out of the tools provided by the Scientific Python community. The second part will cover Jupyter more broadly, including how working with the notebook document format can enable shareable, reproducible analyses. Students should come prepared with the Anaconda Python distribution, or otherwise install common scientific Python tools, such as:

- numpy
- scipy
- pandas
- jupyter
- ipython
- matplotlib
- scikit-learn
- scikit-image

Speaker:

Min Ragan-Kelley, Simula Research Laboratory, Norway

Thursday, March 2

MS69

Recent Advances in Matrix Functions and Applications

10:00 AM-11:40 AM

Room:222

Matrix functions are an increasingly important area of applied mathematics. They are used in a variety of applications including exponential integrators, network analysis, image classification, and computer animation. In addition to the formation of f(A) for dense matrices, much research has focused on computing f(A)b for sparse matrices. The f(A)b problem requires efficient algorithms utilizing matrix--vector products, based on, for, example Krylov subspace methods. In this minisymposium we discuss state-of-the-art algorithms for computing matrix functions, along with recent advances regarding their use in applications.

Organizer: Samuel Relton

University of Manchester, United Kingdom

10:00-10:20 The Radau-Lanczos Method for Matrix Functions

Andreas J. Frommer, Bergische Universität, Germany

10:25-10:45 Block Matrix Formulations for Evolving Networks

Caterina Fenu, RWTH Aachen University, Germany; Desmond Higham, University of Strathclyde, United Kingdom

10:50-11:10 Approximating the Spectral Sums of Large-Scale Matrices using Chebyshev Approximations

Insu Han, KAIST, Korea; Dmitry Malioutov, IBM Research, USA; Haim Avron, Tel Aviv University, Israel; Jinwoo Shin, KAIST, Korea

11:15-11:35 On the Computation of the Action of the Fréchet Derivative

Peter Kandolf, Universität Innsbruck, Austria; Samuel Relton, University of Manchester, United Kingdom

Thursday, March 2

MS195

Computational Plasma Physics - Part I of II

10:00 AM-11:40 AM

Room:Grand Ballroom - 2nd Fl

For Part 2 see MS222

Accurately and efficiently simulating the dynamics of plasma is important in a wide range of applications including astrophysics, space weather, confined fusion, particle accelerators, and semiconductor manufacturing. The simulation of plasma remains a challenging problem due to the great range of temporal and spatial scales inherent in plasma phenomena. This minisymposium addresses recent advances in numerical methods for fluid and kinetic models of plasmas.

Organizer: James A. Rossmanith

Iowa State University, USA

Organizer: David C. Seal

US Naval Academy, USA

10:00-10:20 Positivity-Preserving Hybrid Semi-Lagrangian Discontinuous Galerkin Schemes for the 2D2V Vlasov-Poisson System on Unstructured Meshes

David C. Seal, US Naval Academy, USA; James A. Rossmanith, Iowa State University, USA

10:25-10:45 Solving Fluid and Continuum Kinetic Equations in Plasma Physics Using the Discontinuous Galerkin Method

Bhuvana Srinivasan, Virginia Tech, USA; Ammar Hakim, Princeton Plasma Physics Laboratory, USA; Petr Cagas and Yang Song, Virginia Tech, USA

10:50-11:10 IFP: An Optimal, Adaptive, Fully Conservative and Asymptotic Preserving 1D2V Vlasov-Rosenbluth-Fokker-Planck for Spherical ICF Implosion Calculation

William T. Taitano, Luis Chacon, Andrei Simakov, and Brett Keenan, Los Alamos National Laboratory, USA

11:15-11:35 Comparison of Several Advanced High Order Vlasov Schemes

Wei Guo and Andrew J. Christlieb, Michigan State University, USA

Thursday, March 2

MS196

Compressive Sampling Methods In High-Dimensional Stochastic and Parametric Approximations - Part I of II

10:00 AM-11:40 AM

Room:Ballroom D - 2nd Fl

For Part 2 see MS249

The development of scalable numerical methods for the solution of problems with high-dimensional stochastic or parametric inputs has been a subject of active research in computational sciences and engineering. This is motivated by the need to mitigate the difficulties associated with the rapid growth of computational complexity in the simulation of physical systems where accurate specification of governing equations entails a large number of parameters or stochastic inputs. One such approaches, known as compressive sampling, exploits the sparsity of the quantities of interest (QoI) — in a multivariate basis of inputs — by employing appropriate optimization/regularization techniques. In particular, when sufficiently sparse, the QoI may be accurately computed from a number of its random realizations that depends linearly on the sparsity, as opposed to the cardinality of the basis. This minisymposium presents state-of-the-art in compressive sampling developments for various aspects of high-dimensional computation, including analysis, algorithms, implementation, and applications.

Organizer: Alireza Doostan

University of Colorado Boulder, USA

Organizer: Dongbin Xiu

University of Utah, USA

10:00-10:20 Error Correction for Multivariate Function Approximation

Yeonjong Shin and Dongbin Xiu, Ohio State University, USA

continued on next page

10:25-10:45 High-Dimensional Approximation and Structured Sparsity
Ben Adcock, Yi Sui, and Casie Bao, Simon Fraser University, Canada

10:50-11:10 New Sufficient Conditions for Sparse Recovery via Nonconvex Minimizations
Clayton G. Webster and Hoang A. Tran, Oak Ridge National Laboratory, USA

11:15-11:35 Model Order Reduction and Sparse Approximations for Dynamical Systems with Random Parameters
Roland Pulch, University of Greifswald, Germany

Thursday, March 2

MS197

Nonlocal Models in Computational Science and Engineering - Part I of III

10:00 AM-11:40 AM

Room:202

For Part 2 see MS223

Nonlocal models provide a new framework to overcome limitations and challenges present in classical PDE-based models. For instance, peridynamics, a nonlocal extension of classical continuum mechanics, admits discontinuous solutions and naturally describes material failure and damage. Similarly, nonlocal and fractional diffusion models can represent anomalous diffusion and heat transfer. Furthermore, nonlocal models introduce length scales, which can be used for multiscale modeling. Recent years have witnessed a tremendous advance in modeling, mathematical analysis, and computational practice for nonlocal problems. This minisymposium focuses on recent developments in peridynamics, nonlocal and fractional diffusion, and other related nonlocal models.

Organizer: Marta D'Elia
Sandia National Laboratories, USA

Organizer: Qiang Du
Columbia University, USA

Organizer: Pablo Seleson
Oak Ridge National Laboratory, USA

10:00-10:20 Material Stability and Numerical Stability in Peridynamics
Stewart Silling, Sandia National Laboratories, USA

10:25-10:45 Double Well Potentials and Nonlocal Brittle Fracture Modeling
Robert P. Lipton, Louisiana State University, USA

10:50-11:10 Optimization-Based Coupling for Local and Nonlocal Models
David Littlewood, Marta D'Elia, Mauro Perego, and Pavel Bochev, Sandia National Laboratories, USA

11:15-11:35 A Model for the Transport of Miscible Fluids in the Presence of Anomalous Diffusion
John Foster, University of Texas at Austin, USA

Thursday, March 2

MS198

Numerical Methods for Uncertainty Quantification, Surrogate Models, and Bayesian Inference - Part I of III

10:00 AM-11:40 AM

Room:203

For Part 2 see MS224

It is increasingly important to equip a numerical model or simulation with estimates of uncertainty. For these estimates to be meaningful, they must be carefully derived, e.g., by Bayes' rule and conditional probability, which allows one to estimate model uncertainties from noisy data. Numerical methods to perform such Bayesian inference often rely on Monte Carlo sampling. The cost if these methods can be high, because they require repeated evaluation of a numerical model, where each evaluation may be computationally expensive. This session focuses on techniques that aim to mitigate this computational burden, including replacing high-fidelity models with surrogate models, reducing the dimensionality of the parameter space, devising efficient sampling methods, and employing goal-oriented approaches.

Organizer: Matthias Morzfeld
Lawrence Berkeley National Laboratory, USA

Organizer: Fei Lu
Lawrence Berkeley National Laboratory, USA

Organizer: Kevin T. Carlberg
Sandia National Laboratories, USA

10:00-10:20 Approximate Marginal MCMC for Goal-Oriented Inference with Expensive Models
Andrew D. Davis, Massachusetts Institute of Technology, USA; Natesh Pillai, Harvard University, USA; Aaron Smith, University of Ottawa, Canada; Youssef M. Marzouk, Massachusetts Institute of Technology, USA

continued on next page

Thursday, March 2

MS198

Numerical Methods for Uncertainty Quantification, Surrogate Models, and Bayesian Inference - Part I of III

10:00 AM-11:40 AM

continued

10:25-10:45 Sequential Implicit Sampling Methods for Bayesian Inverse Problems

Xuemin Tu, University of Kansas, USA

10:50-11:10 Improving the Efficiency of Implicit Sampling Using Surrogate Models

George Shu Heng Pau and Yaning Liu, Lawrence Berkeley National Laboratory, USA

11:15-11:35 Aspects of Particle Filtering in Very High Dimensional Systems

Peter Jan van Leeuwen, University of Reading, United Kingdom

Thursday, March 2

MS200

High-Performance Streaming Graph Analysis - Part I of II

10:00 AM-11:40 AM

Room:205

For Part 2 see MS226

Graph analysis extracts information from relationship data prevalent in network security, health informatics, finance, and many other fields. The modeled relationships change over time, sometimes very rapidly. Repeatedly re-analyzing massive graphs often does not keep up with performance requirements. Applications that monitor and respond to data streams can have low latency requirements. For example, analyzing a 10 gigabit Ethernet in real time requires handling over 130,000 network flows per second or an average latency of under 7.7 microseconds. New algorithms and systems can leverage scattered, local changes in this streaming data for rapid response. Less latency-intensive environments also benefit from more focused analysis and higher performance. This minisymposium surveys a range of practical algorithms, software systems, and new directions for analyzing real-world streaming graph data.

Organizer: Jason Riedy

Georgia Institute of Technology, USA

Organizer: Henning Meyerhenke

Karlsruhe Institute of Technology, Germany

10:00-10:20 High-Performance Analysis of Streaming Graphs

Jason Riedy, Georgia Institute of Technology, USA

10:25-10:45 Dense Subgraphs in Temporal Networks: Algorithms and Analysis

A. Erdem Sariyuce and Ali Pinar, Sandia National Laboratories, USA

continued in next column

10:50-11:10 Time-Evolving Graph Processing on Commodity Clusters

Anand Iyer and Ion Stoica, University of California, Berkeley, USA

11:15-11:35 Parallel and Streaming Methods for Real-Time Analysis of Dense Structures from Graphs

Srikanta Tirthapura, Apurba Das, A. Pavan, and Michael Svendsen, Iowa State University, USA; Kanat Tangwongsan, Mahidol University International College, Thailand; Kung-Lun Wu, IBM T.J. Watson Research Center, USA

Thursday, March 2

MS201

PDE-Constrained Optimal Control Under Uncertainty - Part I of II

10:00 AM-11:40 AM

Room:206

For Part 2 see MS227

PDE-constrained optimal control under uncertainty has recently emerged as an important research field. Uncertainties arising from various sources such as computational domains, boundary/initial conditions, material properties, and external loadings are inevitable in practice and have to be taken into consideration for the solution of PDE-constrained optimal control problems. Several computational challenges are faced in solving such problems: one is the curse of dimensionality entailed in high/infinite-dimensional uncertainty, and another is the expensive function evaluations which require PDE solves. The minisymposium will present advances in numerical methods, mathematical analyses and applications aimed at tackling these computational challenges.

Organizer: Peng Chen

University of Texas at Austin, USA

Organizer: Omar Ghattas

University of Texas at Austin, USA

Organizer: Georg Stadler

Courant Institute of Mathematical Sciences, New York University, USA

10:00-10:20 Scalable Methods for Optimization of Systems Governed by PDEs with Random Parameter Fields

Alen Alexanderian, North Carolina State University, USA; Noemi Petra, University of California, Merced, USA; Georg Stadler, Courant Institute of Mathematical Sciences, New York University, USA; Omar Ghattas, University of Texas at Austin, USA

continued in next column

10:25-10:45 Low Rank Solvers for PDE-Constrained Optimization with Uncertain Parameters

Martin Stoll, Max Planck Institute, Magdeburg, Germany; Peter Benner, Max Planck Institute for Dynamics of Complex Technical Systems, Germany; Sergey Dolgov, University of Bath, United Kingdom; Akwum Onwunta, Max Planck Institute, Magdeburg, Germany

10:50-11:10 Multifidelity Computation of Failure Probabilities for Systems with Uncertain Parameters

Boris Kramer, Karen E. Willcox, and Benjamin Peherstorfer, Massachusetts Institute of Technology, USA

11:15-11:35 Multilevel Monte Carlo Analysis for Optimal Control of Elliptic PDEs with Random Coefficients

Ahmad Ahmad Ali and Michael Hinze, Universitat Hamburg, Germany; *Elisabeth Ullmann*, Technische Universität München, Germany

Thursday, March 2

MS202

Quadrature Methods for Singular and Nearly Singular Integrals in Integral Equations - Part I of II

10:00 AM-11:40 AM

Room:209

For Part 2 see MS228

One of the main challenges for integral equation based numerical methods is the numerical integration of singular and nearly singular integrals. This minisymposium will focus on efforts to design accurate quadrature methods that can be efficiently applied for integrals over 3D surfaces.

Organizer: Anna-Karin Tornberg

KTH Royal Institute of Technology, Sweden

10:00-10:20 Expansion Mechanisms for Volume and Layer Potentials in Quadrature By Expansion

Andreas Kloeckner, University of Illinois, USA

10:25-10:45 Deriving Estimates for the Quadrature Error in Quadrature by Expansion (QBX)

Ludvig af Klinteberg, KTH Royal Institute of Technology, Sweden

10:50-11:10 Accurate Derivative Evaluation for Grad-Shafranov Solvers Using Quadrature by Expansion (QBX)

Manas N. Rachh, Yale University, USA; Lee F. Ricketson, and Antoine Cerfon, Courant Institute of Mathematical Science, New York University, USA; Jeffrey Freidberg, Massachusetts Institute of Technology, USA

11:15-11:35 A Local Target-Specific QBX Method for Laplace's Equation in 3D Multiply-Connected Domains

Michael Siegel, New Jersey Institute of Technology, USA

Thursday, March 2

MS203

Programming Challenges for Portable Performance on Heterogeneous Architectures

10:00 AM-11:40 AM

Room:210

DOE reports make it clear that the programming paradigm required for exascale computing must simultaneously solve two very difficult problems: expressing and efficiently utilizing unprecedented parallelism across a massive collection of heterogeneous devices, while also preserving the productivity of application developers. In this minisymposium, we propose to present the view from leading scientists on how to addresses these issues using runtime system and data flow representations to express and manage extreme-scale parallelism, while maintaining the performance portability of the code on heterogeneous system such as GPU and/or KNL.

Organizer: George Bosilca

University of Tennessee, Knoxville, USA

10:00-10:20 Programming Model, Performance Analysis and Optimization Techniques for the Intel Knights Landing Xeon Phi

Azzam Haidar, University of Tennessee, USA; Stanimire Tomov, University of Tennessee, Knoxville, USA; Konstantin Arturov, Murat E. Guney, and Shane Story, Intel Corporation, USA; Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA; *Tyler McDaniel*, University of Tennessee, USA

10:25-10:45 A Comprehensive Study of Differences Between Sequential Task Flow and a Real Data Flow Representation

George Bosilca and Thomas Herault, University of Tennessee, Knoxville, USA

10:50-11:10 Using Kokkos for Performance Portability of the Tpetra Sparse Linear Algebra Library on Intel KNL and Nvidia GPUs

Mark Hoemmen, Sandia National Laboratories, USA

11:15-11:35 Overview of a Sequential Task Flow Sparse QR Multifrontal Solver

Emmanuel Agullo, Inria, France; Alfredo Buttari, CNRS, France; Abdou Guermouche, LaBRI, France; *Ian Masliah,* University of Paris-Sud, France

Thursday, March 2

MS204

Theory, Applications and Numerics for Sturm-Liouville Problems

10:00 AM-11:40 AM

Room:211

The development of software for spectral quantities associated with Sturm-Liouville problems (Eigenvalues, Eigenfunctions, Spectral Density Functions), as well as new areas of application for such software, continues to receive much attention. This Minisymposium will focus on underlying theory for new numerical algorithms, new applications where computed spectral quantities are needed, and new codes.

Organizer: Charles T. Fulton

Florida Institute of Technology, USA

10:00-10:20 Spectral Density Functions for Periodic Schrödinger Potentials

Charles T. Fulton, Florida Institute of Technology, USA; Steven Pruess, Colorado School of Mines, USA; David Pearson, University of Hull, United Kingdom

10:25-10:45 Eigenvalues of Sturm-Liouville Problems with Real Coupled Boundary Conditions

Paul B. Bailey and Anton Zettl, Northern Illinois University, USA

10:50-11:10 Spectral Density Functions Associated with Fokker-Planck Collisions

Rockford D. Foster and Jon Wilkening, University of California, Berkeley, USA

11:15-11:35 Spectral Pollution Arising in Eigenvalue Computations for Schroedinger Operators

Sabine Boegli, Technische Universität München, Germany; Marco Marletta, Cardiff University, United Kingdom; Christiane Tretter and Petr Siegl, University of Bern, Switzerland

Thursday, March 2

MS205

LES Modeling of Turbulence: Methods, Analysis and Applications

10:00 AM-11:40 AM

Room:212

Reliable and efficient turbulence modeling is challenging scientists since decades. The massive use of numerical modes in fields like medicine raises the challenge: modeling of high convective fields is critical in the quantitative analysis of pathologies like aortic diseases. Large Eddie Simulation approach is the most appropriate, yet many questions require specific investigations: modeling choices, parameter sensitivity, accuracy analysis, efficient implementation. This Minisymposium considers different aspects from theory to practical implementation. Comparing theoretical and practical perspectives will significantly advance the knowledge toward a rigorous development of computational tools with a strong impact on old and new applications. Supported by NSF.

Organizer: Alessandro Veneziani

Emory University, USA

Organizer: Annalisa Quaini

University of Houston, USA

10:00-10:20 Large Eddy Simulation of Aortic Flow Using Deconvolution-Based Nonlinear Filter -- Theory and Application

Huijuan Xu, Georgia Institute of Technology, USA; Marina Piccinelli and Bradley Leshnower, Emory University, USA; Luca Bertagna, Florida State University, USA; Annalisa Quaini, University of Houston, USA; Robert Nerem, Georgia Institute of Technology, USA; Alessandro Veneziani, Emory University, USA

continued on next page

10:25-10:45 The Reduced Nsalpha Model for Turbulent Channel Flow
Camille Zerfas, Clemson University, USA

10:50-11:10 Simulation of Flow in Artificial Blood Pumps: Turbulence Modeling and Consideration of Blood Microstructure
Marek Behr, RWTH Aachen University, Germany

11:15-11:35 On the Asymptotic Behavior of Subgrid Scale Models for Large-Eddy Simulations in Complex Geometries
Franck Nicoud, University of Montpellier, France

Thursday, March 2

MS206

Topology Optimization: Formulations, Methods and Applications - Part I of II

10:00 AM-11:40 AM

Room:213

For Part 2 see MS232

Topology optimization is a computational methodology for distributing two or more materials in a given design domain by minimizing a selected objective subject to physical constraints (e.g. compliance minimization subject to weight constraint). Initially applied to problems mainly in structural mechanics the methodology has been utilized in a number of other fields such as microelectromechanical systems, photonics, acoustics and fluid mechanics. Topology optimization is well accepted in industrial design processes where it can provide competitive designs in terms of cost, materials and functionality under a wide set of constraints. The methodology is typically implemented as a PDE constrained optimization problem which presents a number of mathematical challenges, including numerical methods for optimization, fast PDE solvers, and optimization formulations. Therefore, the minisymposium aims to explore these topics and present topology optimization approaches in a range of application spaces.

Organizer: Eric C. Cyr
Sandia National Laboratories, USA

Organizer: Boyan S. Lazarov
Technical University of Denmark, Denmark

10:00-10:20 Design Sensitivities in Topology Optimization via Automatic Differentiation
Boyan S. Lazarov and Sebastian Noergaard, Technical University of Denmark, Denmark

continued in next column

10:25-10:45 Algorithms for the Topology Optimization of Electrical Conductors
Gregory J. von Winckel, Sandia National Laboratories, USA

10:50-11:10 Stochastic Sampling for Structural Topology Optimization with Many Load Cases: Density-Based and Ground Structure Approaches
Xiaojia Zhang, Georgia Institute of Technology, USA; Eric De Sturler, Virginia Tech, USA; Glaucio Paulino, Georgia Institute of Technology, USA

11:15-11:35 Using a Fully Non-Conformal Geometry Description to Enable Optimization-Based Design
Joshua Robbins, Sandia National Laboratories, USA

Thursday, March 2

MS207

Meshless, Particle, and Particle-Mesh Methods for PDEs - Part I of II

10:00 AM-11:40 AM

Room:214

For Part 2 see MS233

Due to their inherent scalability, meshless, particle-based and particle-mesh methods are becoming increasingly important with recent increases in available computing power. Meshless and particle-based methods provide adaptive solutions for problems with deforming interfaces, without the burden of generating boundary conforming meshes. Particle and particle- mesh methods become critically important as scientific and engineering applications move towards more resolved / first principles approaches. In addition to classical applications of particle methods for PDEs in electromagnetism and cosmology, new applications in climate, energy, and environmental areas are adopting particle and hybrid methods. We focus on recent developments using these methods to scalably solve PDEs with diverse applications to scientific and engineering problems. In particular, a spectrum of methods will be represented: Lagrangian particle methods for hydrodynamic problems, recent advances in smoothed particle hydrodynamics, staggered moving least squares, PIC methods for plasma physics problems, as well as topics from scattered data approximation theory. Research issues of particular interest include rigorous foundations of methods based on mathematical approximation theory, error analysis and convergence, improved kernels and high order methods, spatial and temporal adaptivity, and scalability on modern supercomputer architectures.

Organizer: Nathaniel Trask

Sandia National Laboratories, USA

Organizer: Alexander Tartakovsky

Pacific Northwest National Laboratory, USA

10:00-10:20 High-Order Staggered Moving Least Squares Schemes for the Steady Stokes with Applications to Suspension Flows

Nathaniel Trask, Sandia National Laboratories, USA

10:25-10:45 Advances in Smoothed Particle Hydrodynamics

Louis F. Rossi, University of Delaware, USA; Zhenyu He, W. L. Gore & Associates

10:50-11:10 Predicting Cavitation in Fuel Injectors using Smoothed Particle Hydrodynamics

Emily Ryan, Boston University, USA

11:15-11:35 Localized Kernel Methods for Nonlocal Diffusion

Stephen Rowe and Richard B. Lehoucq, Sandia National Laboratories, USA; Joseph Ward and Francis J. Narcowich, Texas A&M University, USA

continued in next column

Thursday, March 2

MS208

Evolution of Co-Design and Scientific HPC Applications - Part I of II

10:00 AM-11:40 AM

Room:215

For Part 2 see MS234

Modernizing scientific codes to run performantly on multiple emerging architectures is a task of great complexity and challenge for computational scientists today. It is typical the set of performance necessary optimizations for a code on a given platform will be distinct from those for another. To ameliorate this difficulty, we turn to abstraction layers and alternative programming models. This minisymposium will present the integrations of small-scale experiments into production level codes, programming models and runtimes which support them, and other research towards next-generation scientific HPC applications.

Organizer: Geoff Womeldorff

Los Alamos National Laboratory, USA

Organizer: Ian Karlin

Lawrence Livermore National Laboratory, USA

10:00-10:20 Adapting Proxy Lessons Learned to Integrate C++ Kokkos into a Production Fortran Code

Joshua Payne, Geoff Womeldorff, and Ben Bergen, Los Alamos National Laboratory, USA

10:25-10:45 Experiences with Kokkos in the Production Codebases

Simon D. Hammond, Sandia National Laboratories, USA

10:50-11:10 Performance Portable Production Hydrodynamics Using Raja and Chai

Peter Robinson, Lawrence Livermore National Laboratory, USA

11:15-11:35 Targeting Next-Generation Software Stacks with the Nabla DSL

Jean-Sylvain Camier, CEA, DAM, DIF, France

Thursday, March 2

MS209

Coarse-Graining, Stochastic Parametrizations and the Mori-Zwanzig Formulation - Part I of II

10:00 AM-11:40 AM

Room:216

For Part 2 see MS235

Microscopic simulations based on interacting particles are becoming increasingly prevalent in the modeling of complex systems such as those in material science, biology and soft matter physics. One of the main objectives of such simulations is understand large-scale effects based on microscopic first principles. The computational cost of particle-based simulations depends critically on the number of particles and the interaction potentials, and can require hundred of thousands of computer cores and significant computing time and data processing to be successfully completed. This motivates the use of coarse-graining techniques such as the Mori-Zwanzig formulation to compute macroscopic/mesoscopic observables at a reasonable computational cost. This minisymposium invites contributions that showcase the potential and effectiveness of coarse-graining techniques in applied sciences, including particle models and multi-scale stochastic dynamical systems.

Organizer: Jason Dominy
University of California, Santa Cruz, USA

10:00-10:20 Non-Isothermal Coarse-Graining of Complex Molecules
Pep Español, Universidad Nacional de Educación a Distancia, Spain

10:25-10:45 On Memory Estimation in the Mori-Zwanzig Equation
Yuanran Zhu, Jason Dominy, and Daniele Venturi, University of California, Santa Cruz, USA

10:50-11:10 Coupling a Nano-Particle with Fluctuating Hydrodynamics
Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA; Pep Espa\~nol, Universidad Nacional de Educación a Distancia, Spain

11:15-11:35 Investigation of the Molecular Aspects of Fluctuating Hydrodynamics Through the Memory Function Approach
Changho Kim, Lawrence Berkeley National Laboratory, USA

continued in next column

Thursday, March 2

MS210

Tensor Decompositions: Applications and Efficient Algorithms - Part I of II

10:00 AM-11:40 AM

Room:217

For Part 2 see MS236

Tensors, or multidimensional arrays, are a natural way to represent high-dimensional data arising in a multitude of applications. Tensor decompositions, such as the CANDECOMP/PARAFAC and Tucker models, help to identify latent structure, achieve data compression, and enable other tools of data analysis. This minisymposium identifies pressing applications for multidimensional data analysis as well as efficient algorithms for computing various tensor decompositions.

Organizer: Grey Ballard
Wake Forest University, USA

Organizer: Tamara G. Kolda
Sandia National Laboratories, USA

Organizer: Bora Ucar
LIP-ENS Lyon, France

10:00-10:20 Discovering Fast Matrix Multiplication Algorithms Via Tensor Decomposition
Grey Ballard, Wake Forest University, USA

10:25-10:45 A Practical Randomized CP Tensor Decomposition
Casey Battaglino, Georgia Institute of Technology, USA

10:50-11:10 Tensor Based Approaches in Magnetic Resonance Spectroscopic Signal Analysis
Bharath Halandur Nagaraja, Diana Sima, and *Sabine Van Huffel*, KU Leuven, Belgium

11:15-11:35 Fast Recompression of Hadamard Products of Tensors
Daniel Kressner, École Polytechnique Fédérale de Lausanne, Switzerland; Lana Perisa, University of Split, Croatia

Thursday, March 2

MS211

Algorithmic Revolution in Post Moore's Era: Auto-Tuning and Accuracy Assurance - Part I of II

10:00 AM-11:40 AM

Room:218

For Part 2 see MS237

It is expected that by the end of 2020 no gains in FLOPS counting will be achieved with a constant power budget due to physical limitations in device miniaturization. This inflection point, referred to as "Post Moore's Era", is already leading researchers to consider that the ability to memory access (BYTES) is becoming more relevant than a growing FLOPS. Hence, an algorithmic revolution, from FLOPS to BYTES, will be necessary for efficient numerical computations. We believe that auto-tuning (AT) technologies will be built upon it is proven success path, and have the ability of providing optimized, high performance implementations of specific computations for architectures of the Post Moore's Era. It is expected that these architectures will enable the solution of problems with unprecedented levels of details, implying very large problems, which in turn raises concerns about the accuracy of the computations. Usually, codes that perform floating point sums of distributed data cannot expect the results to be reproducible. This is likely to be exacerbated in the Post Moore's Era; thus an increasing interest about how to address nonreproducibility in large applications. This minisymposium will discuss technologies for AT and its interplay with accuracy assurance towards the Post Moore's Era.

Organizer: Takahiro Katagiri

Nagoya University, Japan

Organizer: Toshiyuki Imamura

RIKEN Advanced Institute for Computational Science, Japan

continued in next column

Organizer: Osni A. Marques

Lawrence Berkeley National Laboratory, USA

10:00-10:20 Algorithmic Revolution and Auto-Tuning for Matrix Computations in Post Moore's Era

Takahiro Katagiri, Nagoya University, Japan; Satoshi Ohshima and Masaharu Matsumoto, University of Tokyo, Japan

10:25-10:45 Speed vs. Accuracy: The Next Frontier for Auto-Tuning?

Jeffery Hollingsworth, University of Maryland, USA

10:50-11:10 A Directive-Based Data Layout Auto-Tuning for OpenACC Applications

Tetsuya Hoshino, University of Tokyo, Japan; Naoya Maruyama, RIKEN, Japan; Satoshi Matsuoka, Tokyo Institute of Technology, Japan

11:15-11:35 User-Defined Directive Translation Using the Xevovler Framework

Kazuhiko Komatsu, Ryusuke Egawa, Hiroyuki Takizawa, and Hiroaki Kobayashi, Tohoku University, Japan

Thursday, March 2

MS212

Recent Developments in Linear System Solvers Based on Low-Rank Approximation Techniques - Part I of II

10:00 AM-11:40 AM

Room:219

For Part 2 see MS238

The primary goal of this minisymposium is to discuss recent developments in linear system solvers based on low-rank approximation techniques. Low-rank approximation techniques have drawn much attention in recent years and led to much progress in developing more efficient methods for solving large scale linear systems. These techniques resulted in fast direct solvers based on (nearly) linear time matrix factorizations or inversions and robust preconditioners for indefinite and ill-conditioned systems. All the 8 presentations in this minisymposium have shown relevant and of great importance to this topic. The applications ranges from PDEs, integral equations, machine learning applications, etc.

Organizer: Yuanzhe Xi

University of Minnesota, USA

Organizer: Ruipeng Li

Lawrence Livermore National Laboratory, USA

10:00-10:20 Divide-and-Conquer Approximate Inverse Type and Schur Complement Based Preconditioners with Low-Rank Corrections

Ruipeng Li, Lawrence Livermore National Laboratory, USA

10:25-10:45 Developing Preconditioners with Guaranteed Convergence Rate Using Hierarchical Matrices

Eric F. Darve, Chao Chen, Hadi Pouransari, and Kai Yang, Stanford University, USA

10:50-11:10 A Cache-Efficient Rank-Structured Elliptic PDE Solver

David Bindel, Cornell University, USA

11:15-11:35 Distributed-Memory Hierarchical Interpolative Factorization

Yingzhou Li and Lexing Ying, Stanford University, USA

Thursday, March 2

MS213

Science and Engineering Applications of Derivative-Free Optimization - Part I of II

10:00 AM-11:40 AM

Room:220

For Part 2 see MS239

Numerical optimization arises throughout computational science and engineering, from design optimization and optimal control to model calibration and data assimilation. This minisymposium concerns settings where some derivatives of the objective function and/or constraints are unavailable or otherwise unreliable. The talks will address a diverse set of challenges that arise in different applications and will highlight how these challenges pose problem for classical optimization methods. Presented will be recent algorithmic and computational advances that enable solution of difficult science and engineering problems that were previously out of reach.

Organizer: Stefan Wild

Argonne National Laboratory, USA

10:00-10:20 Optimizing the Design of Concentrated Solar Power Plants

Jeffrey Larson and Sven Leyffer, Argonne National Laboratory, USA; Michael Wagner, National Renewable Energy Laboratory, USA

10:25-10:45 Bayesian Optimization under Mixed Constraints with a Slack-Variable Augmented Lagrangian

Victor Picheny, Inria, France; Robert Gramacy, Virginia Tech, USA; Stefan Wild, Argonne National Laboratory, USA

10:50-11:10 A Hybrid Mixed-Integer Approach to Design Basin Networks for Water Resources Management

Kathleen Kavanagh, Clarkson University, USA

11:15-11:35 Three Dimensional Variational Data Assimilation Based on Derivative-Free Optimization

Elias Niño-Ruiz, Universidad del Norte, Colombia; Adrian Sandu, Virginia Tech, USA

Thursday, March 2

MS214

Parallel Implementations of Hierarchical Matrix-based Algorithms - Part I of II

10:00 AM-11:40 AM

Room:Crystal AF - 1st Fl

For Part 2 see MS240

In the last two decades, there have been substantial theoretical and practical advances in the area of fast direct solvers, often relying on hierarchical low-rank approximations in its different data-sparse formats. Leveraging these contributions is most needed today as computer hardware changes rapidly and the need to solve relevant problems efficiently is ever present. This minisymposium focuses on the synergies between theory and practical implementations of a variety of algorithms that by exploiting a hierarchy of low-rank approximations deliver optimal complexity scalable solvers for relevant problems in science and engineering.

Organizer: Pieter Ghysels

Lawrence Berkeley National Laboratory, USA

Organizer: Gustavo Chavez

King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: David E. Keyes

King Abdullah University of Science & Technology (KAUST), Saudi Arabia

10:00-10:20 Accelerated Cyclic Reduction (ACR): A Distributed Memory Fast Direct Solver for 3D Structured Linear Systems

Gustavo Chavez, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; George M Turkiyyah, American University of Beirut, Lebanon; Hatem Ltaief and David E. Keyes, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

10:25-10:45 Distributed-Memory Hierarchical Matrix Algebra

Yingzhou Li, Jack L. Poulson, and Lexing Ying, Stanford University, USA

continued in next column

10:50-11:10 Parallel Hierarchical Solvers, Convergence for Large Mesh Sizes

Chao Chen, Stanford University, USA; Siva Rajamanickam and Erik G. Boman, Sandia National Laboratories, USA; Eric F. Darve, Stanford University, USA

11:15-11:35 Preconditioning using Hierarchically Semi-Separable Matrices and Randomized Projection

Pieter Ghysels and X. Sherry Li, Lawrence Berkeley National Laboratory, USA; Francois-Henry Rouet, Livermore Software Technology Corporation, USA; Chris Gorman, University of California, Santa Barbara, USA

Thursday, March 2

MS215

New Approaches to Complex Coupled Multiscale Systems - Part I of II

10:00 AM-11:40 AM

Room:Crystal CD - 1st Fl

For Part 2 see MS241

As the fidelity of computational algorithms increases, and the computational resources (hardware and software simulation systems) become more available, computational and applied mathematics can now simulate a variety of complex coupled phenomena with multiple scales which were unfeasible a decade ago. However, the complexity of real world and the availability of data poses new challenges in order to move beyond the proof-of-concept realizations and closer to the goal of describing and managing real-life applications with meaningful objectives. In this minisymposium the presentations will describe novel modeling and algorithmic approaches which can work with, and interpret real data.

Organizer: Malgorzata Peszynska

Oregon State University, USA

10:00-10:20 Multiscale Models of Sea Ice

Kenneth M. Golden, University of Utah, USA

10:25-10:45 Multiscale Modeling in Coastal Ocean Hydrodynamics

Clint Dawson, University of Texas at Austin, USA

10:50-11:10 A Mathematical and Geological Approach for Fractured Geothermal System

Alessio Fumagalli and Eirik Keilegavlen, University of Bergen, Norway

11:15-11:35 Multiphysics Modeling of Microseismic Events for Elastic Wavefield Synthesis

Susan Minkoff, Matthew McChesney, and George McMechan, University of Texas at Dallas, USA

Thursday, March 2

MS216

Flow-Induced Shaping Processes: Erosion, Dissolution, Ablation, and Phase Change - Part I of II

10:00 AM-11:40 AM

Room:301

For Part 2 see MS242

All around us, solid material is shaped, transported, and obliterated by flowing fluids, from soil and sediment on Earth's surface to plaque within human arteries. These material-removal processes - including erosion, dissolution, ablation, and melting - will be the focus of this special session. Particular emphasis will be placed on geophysical examples and on viewing these processes from the moving-boundary-problem perspective. The session will feature theoretical modeling and numerical simulations, as well as laboratory experiments and field measurements. It will bring together scientists and mathematicians from a range of backgrounds.

Organizer: Matthew N. Moore

Florida State University, USA

Organizer: Bryan D. Quaife

Florida State University, USA

10:00-10:20 How Bodies Erode and Dissolve in Fluid Flows

Nick Moore, Florida State University, USA

10:25-10:45 Curvature Driven Erosion and Channelization of Sedimentary Beds by Fluid Flow

Arshad Kudrolli, Clark University, USA

10:50-11:10 Viscous Erosion of Immersed Bodies at Low and Intermediate Reynolds Numbers

Saverio E. Spagnolie, University of Wisconsin, USA

11:15-11:35 Geometry of Channel Networks Incised by Subsurface Flow

Daniel Rothman and Yossi Cohen, Massachusetts Institute of Technology, USA; Olivier Devauchelle, Institut de Physique du Globe de Paris, France; Hansjoerg Seybold, ETH Zürich, Switzerland; Robert Yi, Massachusetts Institute of Technology, USA

Thursday, March 2

MS217

Theoretical and Computational Advancements in Ice Sheet Modeling - Part I of II

10:00 AM-11:40 AM

Room:302

For Part 2 see MS243

Accurately modeling the dynamics of large ice sheets is essential for projections of sea level rise in the 21st century, but faces many mathematical challenges. Ongoing research includes the development of accurate and tractable models for ice sheet dynamics (e.g., models featuring more physically correct temperature effects, boundary conditions, and/or domain movement, etc.), coupling between ice dynamics and other climate components, (e.g., atmosphere, ocean, etc.) necessary for global climate simulations, and data assimilation, to calibrate parameters and/or initial/boundary conditions. This minisymposium addresses advancements in the development of stand-alone and coupled land-ice models, as well as computational strategies to tackle the resulting discrete problems.

Organizer: Luca Bertagna

Florida State University, USA

Organizer: Mauro Perego

Sandia National Laboratories, USA

Organizer: Irina K. Tezaur

Sandia National Laboratories, USA

Organizer: Daniel Martin

Lawrence Berkeley National Laboratory, USA

10:00-10:20 Coupling Between Ice Dynamics and Subglacial Hydroogy

Luca Bertagna, Florida State University, USA; Mauro Perego, Sandia National Laboratories, USA; Max Gunzburger and Konstantin Pieper, Florida State University, USA

continued on next page

10:25-10:45 Implicit Time-Stepping for the Cryosphere
Ed Bueler, University of Alaska, Fairbanks, USA

10:50-11:10 Simulating Sea Ice Interactions with Ice Sheets Though Granular Iceberg M\'{e}lange in a Discrete Element Model
Alexander Robel, California Institute of Technology, USA

11:15-11:35 Ice-Ocean Coupled Modeling with POPSICLES
Daniel Martin, Lawrence Berkeley National Laboratory, USA; Xylar Asay-Davis, Potsdam Institute for Climate Impact Research, Germany

Thursday, March 2

MS218

Advances in Methods with the Summation-by-Parts Property - Part I of II

10:00 AM-11:40 AM

Room:303

For Part 2 see MS244

As we move towards an era of exascale HPC, flexible and robust algorithms will be necessary to take advantage of increasingly complex and failure prone computational resources. In this minisymposium, the focus is on methods having the summation-by-parts (SBP) property, which are advantageous as they lead to high-order methods that are provably conservative and stable. In particular, the interest is in recent advancements leading to improved efficiency, flexibility, and robustness. Topics that will be covered include: Stable and conservative coupling procedures for non- conforming elements and mesh adaptation; Nonlinearly stable algorithms; Discretization of split forms.

Organizer: David C. Del Rey Fernandez
University of Toronto Institute for Aerospace Studies, Canada

Organizer: Jason E. Hicken
Rensselaer Polytechnic Institute, USA

Organizer: Andrew R. Winters
University of Cologne, Germany

10:00-10:20 Dense-Norm Multi-Dimensional Summation-by-Parts Operators
David C. Del Rey Fernandez, University of Toronto Institute for Aerospace Studies, Canada; Jason E. Hicken, Rensselaer Polytechnic Institute, USA; David W. Zingg, University of Toronto, Canada

10:25-10:45 Improved Numerical Performance Using the SBP-SAT Technique As the Main Building Block
Jan Nordström, Linköping University, Sweden

10:50-11:10 Super Convergence of Summation-By Parts Methods
Gunilla Kreiss, Uppsala University, Sweden

11:15-11:35 Stable And Accurate Grid Interfaces For The Dynamic Beam Equation Using Summation By Parts Finite Differences
Jonatan Werpers and Ken Mattsson, Uppsala University, Sweden

Thursday, March 2

MS219

Multiscale Models and Algorithms for Materials Science - Part I of II

10:00 AM-11:40 AM

Room:304

For Part 2 see MS245

Multiscale material models aim to capture highly nonlinear phenomenon arising from molecular-level behavior and its interaction with larger scale materials properties, while vastly reducing the computational costs compared to direct simulation. This minisymposium brings together contributions to the development and analysis of algorithms handling a wide range of problems such as defect-laden materials, non-local behavior, finite temperature effects, and multiscale dynamical interactions.

Organizer: Matthew Dobson
University of Massachusetts, Amherst, USA

Organizer: Xingjie Li
University of North Carolina, Charlotte, USA

10:00-10:20 Seamless Coupling of Nonlocal and Local Models
Yunzhe Tao, Qiang Du, and Xiaochuan Tian, Columbia University, USA

10:25-10:45 Force-Based Atomistic-to-Continuum Coupling Methods for Multilattices Materials
Derek Olson, Rensselaer Polytechnic Institute, USA; Xingjie Li, University of North Carolina, Charlotte, USA; Christoph Ortner, University of Warwick, United Kingdom

10:50-11:10 Blending Methods for Effective Local/Nonlocal Coupling in Materials Modeling
Pablo Seleson, Oak Ridge National Laboratory, USA

11:15-11:35 Computation of Free Energy of Defects in Atomistic Systems
Matthew Dobson, University of Massachusetts, Amherst, USA; Hong Duong and Christoph Ortner, University of Warwick, United Kingdom

Thursday, March 2

MS220

Adaptive Methods for Uncertainty Quantification and Error Estimation - Part I of II

10:00 AM-11:40 AM

Room:305

For Part 2 see MS246

A common goal in scientific computation is to quantify uncertainties and/or estimate errors of specific prediction or input quantities of interest. As computational models become more complex, the dimension of the input/output spaces increase, or the UQ/error estimation method becomes more sophisticated, some form of adaptivity must be employed to circumvent various computational issues arising from finite computational budgets.

Organizer: Jehanzeb H. Chaudhry
University of New Mexico, USA

Organizer: Troy Butler
University of Colorado, Denver, USA

10:00-10:20 Adaptive Construction of Spatially Varying Polynomial Chaos for Uncertainty Quantification in Transport Problems
Eric C. Cyr, Sandia National Laboratories, USA; Jason Li and Assad Oberai, Rensselaer Polytechnic Institute, USA; Eric Phipps, Sandia National Laboratories, USA; Onkar Sahni, Rensselaer Polytechnic Institute, USA

10:25-10:45 Localizing Uncertainty with Gaussian Markov Random Field Models
Hans-Werner Van Wyk, Auburn University, USA

10:50-11:10 Adaptive Measure-Theoretic Augmentation of Multifidelity Monte Carlo Estimation
Lindley C. Graham and Max Gunzburger, Florida State University, USA

11:15-11:35 Error Estimation and Adaptive Error Control in Measure-Theoretic Stochastic Inversion
Steven Mattis, Technische Universität München, Germany; Troy Butler, University of Colorado, Denver, USA

Thursday, March 2

CP15

Computational Geosciences

10:00 AM-11:40 AM

Room:223

Chair: To Be Determined

10:00-10:10 Optimal Reconstruction of Constitutive Relations for Porous Media Flows
Vladislav Bukshtynov, Florida Institute of Technology, USA

10:12-10:22 Domain-Specific Abstractions for Full-Waveform Inversion
Felix J. Herrmann, University of British Columbia, Canada

10:24-10:34 Abstract Framework for Separable FWI Problems
Mario Bencomo and William Symes, Rice University, USA

10:36-10:46 Adaptive BDDC for Flow in Heterogeneous Porous Media
Bedrich Sousedik, University of Maryland, Baltimore County, USA

10:48-10:58 A Finite Element Flow and Transport Model in Porous Media for Enhanced Oil Recovery Tests at Laboratory Scale
Martin A. Diaz-Viera, Instituto Mexicano del Petróleo, México; Eduardo Linares-Perez and Mario Noyola-Rodriguez, Universidad Nacional Autonoma de Mexico, Mexico

11:00-11:10 Multiscale Methods for Flow and Transport in Porous Media
Yerlan Amanbek, Gurpreet Singh, and Mary F. Wheeler, University of Texas at Austin, USA

Thursday, March 2

CP16

Numerical PDEs - Part V of VI

10:00 AM-11:40 AM

Room:224

For Part 4 see CP14
For Part 6 see CP18

Chair: Talea Mayo, University of Central Florida, USA

10:00-10:10 A Fast Direct Solver for Boundary Integral Equations in Evolving 2D Domains
Tianyu Qiu and Adrianna Gillman, Rice University, USA

10:12-10:22 An Implicit Approach to Phase Field Modeling of Solidification for Additively Manufactured Materials
Chris Newman and Marianne M. Francois, Los Alamos National Laboratory, USA

10:24-10:34 Numerical Shape Optimization to Decrease Failure Probability of Ceramic Structures
Camilla Hahn and Matthias Bolten, Universität Kassel, Germany; Hanno Gottschalk, University of Wuppertal, Germany

10:36-10:46 Fluidity Based Approach to Modeling Ice Sheets
Jeffery M. Allen, University of Colorado Boulder, USA

10:48-10:58 Accurate and Stable Time Stepping in Ice Sheet Modeling
Gong Cheng, Per Lötstedt, and Lina von Sydow, Uppsala University, Sweden

11:00-11:10 Hurricane Uncertainty Propagation for Real-Time Storm Surge Forecasting
Talea Mayo, University of Central Florida, USA

Thursday, March 2

IP8

Computational Science and Engineering Achievements in the Designing of Aircraft

11:50 AM-12:35 PM

Room:Grand Ballroom - 2nd Fl

Chair: Remi Abgrall, University of Zurich, Switzerland

This presentation will give an overview of what Computational Science and Engineering has brought in design capacities these last years in the aeronautics industry. The unceasing increase in computing resources and remarkable improvements of solving methods have enabled industry to perform computations that were not conceivable several before. An emphasis will be scoped to optimization methods as actual engineering tools utilized for industrial applications, in particular for aerodynamic shape design. Numerical formulation and implementation issues will be recalled and illustrations of applications will be discussed. The study of efficient multidisciplinary approaches will be also addressed. New field of applications of Computational Science and Engineering have emerged these last years. Stochastic methods are in the process to take more and more an important place in the toolset of the design engineer and beyond. Some examples of application will be given. The presentation will end with the challenges related to Computational Science and Engineering for aeronautical industry.

Bruno Stoufflet
Dassault Aviation, France

Lunch Break

12:35 PM-2:15 PM

Attendees on their own

Thursday, March 2

MT8

Interactive CSE with IPython and Jupyter- Part II

2:15 PM-3:55 PM

Room:Ballroom C - 2nd Fl

For Part 1 see MT7

Chair: Min Ragan-Kelley, Simula Research Laboratory, Norway

IPython and Jupyter provide tools for interactive computing that are widely used in science and education, and can benefit any CSE instructor, student, or researcher. We will show how to use IPython to improve your interactive explorations in Python, and how Jupyter notebooks enable interactive exploration, teaching, learning, and reproducibility, in Python as well as other languages such as MatLab, Julia, and R. The first part of the tutorial will focus on using IPython to get the most out of the tools provided by the Scientific Python community. The second part will cover Jupyter more broadly, including how working with the notebook document format can enable shareable, reproducible analyses. Students should come prepared with the Anaconda Python distribution, or otherwise install common scientific Python tools, such as:

- numpy
- scipy
- pandas
- jupyter
- ipython
- matplotlib
- scikit-learn
- scikit-image

Speaker:

Min Ragan-Kelley, Simula Research Laboratory, Norway

Thursday, March 2

MS86

Methods for Data-driven Uncertainty Quantification of Large-scale Complex Dynamic Systems

2:15 PM-3:55 PM

Room:222

This minisymposium is focused on recent advances and challenges occurring at the confluence of uncertainty quantification and high-performance computing. The overarching focus area is Bayesian approach to state and parameter estimation and prediction of large-scale, realistic systems governed by differential and algebraic systems of equations and informed by modern sensing devices. Emphasis will put on scalable techniques for uncertainty quantification and decision-making (economic optimization, control, design, etc) under uncertainty, with subtopic including stochastic optimization using high-performance computing, spectral estimation, error analysis.

Organizer: Emil M. Constantinescu
Argonne National Laboratory, USA

Organizer: Emil M. Constantinescu
Argonne National Laboratory, USA

Organizer: Cosmin G. Petra
Lawrence Livermore National Laboratory, USA

Organizer: Noemi Petra
University of California, Merced, USA

2:15-2:35 A Bayesian Approach for Inverse Problems in Dynamic Power Systems

Emil M. Constantinescu, Argonne National Laboratory, USA; Noemi Petra, University of California, Merced, USA; Cosmin G. Petra, Lawrence Livermore National Laboratory, USA; Mihai Anitescu, Argonne National Laboratory, USA

continued on next page

Thursday, March 2

MS86

Methods for Data-driven Uncertainty Quantification of Large-scale Complex Dynamic Systems

2:15 PM-3:55 PM

continued

2:40-3:00 Optimization and Design of Complex Engineering Systems under Uncertainty Using High-Performance Computing

Cosmin G. Petra, Lawrence Livermore National Laboratory, USA

3:05-3:25 Probabilistic Density Function Method for Nonlinear Dynamical Systems Driven by Colored Noise

Alexandre M. Tartakovsky and David A. Barajas-Solano, Pacific Northwest National Laboratory, USA

3:30-3:50 Enabling Large-Scale Power Grid Data Assimilation through Computational Enhancements

Henry Huang and Steve Elbert, Pacific Northwest National Laboratory, USA; Ning Zhou, Binghamton University, USA; Shaobu Wang, Pacific Northwest National Laboratory, USA

Thursday, March 2

MS222

Computational Plasma Physics - Part II of II

2:15 PM-3:55 PM

Room:Grand Ballroom - 2nd Fl

For Part 1 see MS195

Accurately and efficiently simulating the dynamics of plasma is important in a wide range of applications including astrophysics, space weather, confined fusion, particle accelerators, and semiconductor manufacturing. The simulation of plasma remains a challenging problem due to the great range of temporal and spatial scales inherent in plasma phenomena. This minisymposium addresses recent advances in numerical methods for fluid and kinetic models of plasmas.

Organizer: James A. Rossmanith

Iowa State University, USA

Organizer: David C. Seal

US Naval Academy, USA

2:15-2:35 A Hybrid DG/Spectral Method for Micro-Macro Partitioned Kinetic Models

James A. Rossmanith, Iowa State University, USA

2:40-3:00 Volume Integral Methods for Waves in Plasmas

Lise-Marie Imbert-Gerard, Courant Institute of Mathematical Sciences, New York University, USA

3:05-3:25 Towards Scalable and Efficient Solution of IMEX Full-Maxwell / Multifluid Plasma Models*

John Shadid, Edward G. Phillips, Eric C. Cyr, Roger Pawlowski, Matthew Bettencourt, Paul Lin, and Sean Miller, Sandia National Laboratories, USA

3:30-3:50 DG Schemes for Collisional Plasma Models with Insulating Conditions on Rough Boundaries

Jose A. Morales Escalante and Irene M. Gamba, University of Texas at Austin, USA

Thursday, March 2

MS223

Nonlocal Models in Computational Science and Engineering - Part II of III

2:15 PM-3:55 PM

Room:202

For Part 1 see MS197
For Part 3 see MS250

Nonlocal models provide a new framework to overcome limitations and challenges present in classical PDE-based models. For instance, peridynamics, a nonlocal extension of classical continuum mechanics, admits discontinuous solutions and naturally describes material failure and damage. Similarly, nonlocal and fractional diffusion models can represent anomalous diffusion and heat transfer. Furthermore, nonlocal models introduce length scales, which can be used for multiscale modeling. Recent years have witnessed a tremendous advance in modeling, mathematical analysis, and computational practice for nonlocal problems. This minisymposium focuses on recent developments in peridynamics, nonlocal and fractional diffusion, and other related nonlocal models.

Organizer: Marta D'Elia

Sandia National Laboratories, USA

Organizer: Qiang Du

Columbia University, USA

Organizer: Pablo Seleson

Oak Ridge National Laboratory, USA

2:15-2:35 Bridging Scales Through Nonlocal Modeling

Qiang Du, Columbia University, USA

2:40-3:00 A Multi-Time-Step Method for Partitioned Time Integration of Peridynamics

Payton Lindsay, Purdue University, USA; *Michael L. Parks*, Sandia National Laboratories, USA; Arun Prakash, Purdue University, USA

3:05-3:25 A Fast Numerical Method for a Linear Peridynamic Model

Hong Wang, University of South Carolina, USA

3:30-3:50 Predictability of Oscillatory Cracks in Glass: A Peridynamic Study

Florin Bobaru, University of Nebraska, Lincoln, USA; Zhanping Xu and Guanfeng Zhang, University of Nebraska, USA

Thursday, March 2

MS224

Numerical Methods for Uncertainty Quantification, Surrogate Models, and Bayesian Inference - Part II of III

2:15 PM-3:55 PM

Room:203

For Part 1 see MS198
For Part 3 see MS251

It is increasingly important to equip a numerical model or simulation with estimates of uncertainty. For these estimates to be meaningful, they must be carefully derived, e.g., by Bayes' rule and conditional probability, which allows one to estimate model uncertainties from noisy data. Numerical methods to perform such Bayesian inference often rely on Monte Carlo sampling. The cost if these methods can be high, because they require repeated evaluation of a numerical model, where each evaluation may be computationally expensive. This session focuses on techniques that aim to mitigate this computational burden, including replacing high-fidelity models with surrogate models, reducing the dimensionality of the parameter space, devising efficient sampling methods, and employing goal-oriented approaches.

Organizer: Matthias Morzfeld

Lawrence Berkeley National Laboratory, USA

Organizer: Fei Lu

Lawrence Berkeley National Laboratory, USA

Organizer: Kevin T. Carlberg

Sandia National Laboratories, USA

2:15-2:35 Fast Hessian Approximation in Bayesian Inverse Wave Propagation

Georg Stadler, Courant Institute of Mathematical Sciences, New York University, USA; Hejun Zhu, Princeton University, USA; Omar Ghattas, University of Texas at Austin, USA

continued in next column

2:40-3:00 Bayesian Inference for Preconditioned Inverse Ice Sheet Problems

Ruanui Nicholson, University of California, Merced, USA; Georg Stadler, Courant Institute of Mathematical Sciences, New York University, USA; Omar Ghattas, University of Texas at Austin, USA; Noemi Petra, University of California, Merced, USA

3:05-3:25 A Unified Framework for Randomized Methods in Large-Scale Inverse Problems

Ellen B. Le and Tan Bui-Thanh, University of Texas at Austin, USA

3:30-3:50 Active Subspaces for Low-Dimensional Response Surfaces on High-Dimensional Parameter Spaces

Paul Constantine, Colorado School of Mines, USA

Thursday, March 2

MS226

High-Performance Streaming Graph Analysis - Part II of II

2:15 PM-3:55 PM

Room:205

For Part 1 see MS200

Graph analysis extracts information from relationship data prevalent in network security, health informatics, finance, and many other fields. The modeled relationships change over time, sometimes very rapidly. Repeatedly re-analyzing massive graphs often does not keep up with performance requirements. Applications that monitor and respond to data streams can have low latency requirements. For example, analyzing a 10 gigabit Ethernet in real time requires handling over 130,000 network flows per second or an average latency of under 7.7 microseconds. New algorithms and systems can leverage scattered, local changes in this streaming data for rapid response. Less latency-intensive environments also benefit from more focused analysis and higher performance. This minisymposium surveys a range of practical algorithms, software systems, and new directions for analyzing real-world streaming graph data.

Organizer: Jason Riedy

Georgia Institute of Technology, USA

Organizer: Henning Meyerhenke

Karlsruhe Institute of Technology, Germany

2:15-2:35 On Betweenness Centrality Problems in Dynamic Graphs

Elisabetta Bergamini and Henning Meyerhenk, Karlsruhe Institute of Technology, Germany

2:40-3:00 Predicting Movement of Vertices Across Communities in Dynamic Networks

Sriram Srinivasan and Sanjukta Bhowmick, University of Nebraska, Omaha, USA

3:05-3:25 Large-Scale Dynamic Graph Processing on HPC Systems

Keita Iwabuchi, Tokyo Institute of Technology, Japan; Roger Pearce, Texas A&M University, USA; Maya Gokhale, Lawrence Livermore National Laboratory, USA; Satoshi Matsuoka, Tokyo Institute of Technology, Japan

3:30-3:50 Creating Dynamic Graphs from Temporal Data

Anita Zakrzewska, Georgia Institute of Technology, USA

Thursday, March 2

MS227

PDE-Constrained Optimal Control Under Uncertainty - Part II of II

2:15 PM-3:55 PM

Room:206

For Part 1 see MS201

PDE-constrained optimal control under uncertainty has recently emerged as an important research field. Uncertainties arising from various sources such as computational domains, boundary/initial conditions, material properties, and external loadings are inevitable in practice and have to be taken into consideration for the solution of PDE-constrained optimal control problems. Several computational challenges are faced in solving such problems: one is the curse of dimensionality entailed in high/infinite-dimensional uncertainty, and another is the expensive function evaluations which require PDE solves. The minisymposium will present advances in numerical methods, mathematical analyses and applications aimed at tackling these computational challenges.

Organizer: Peng Chen

University of Texas at Austin, USA

Organizer: Omar Ghattas

University of Texas at Austin, USA

Organizer: Georg Stadler

Courant Institute of Mathematical Sciences, New York University, USA

2:15-2:35 Adaptive Methods for PDE Constrained Optimization with Uncertain Data

Matthias Heinkenschloss, Rice University, USA

2:40-3:00 Uncertainty Regions in Shape Optimization

Volker H. Schulz and Martin Siebenborn, University of Trier, Germany

3:05-3:25 On the Efficient Treatment of Uncertainties Within Optimization Problems

Claudia Schillings, University of Warwick, United Kingdom

3:30-3:50 DDM for Stochastic Problems

Jangwoon Lee, University of Mary Washington, USA

Thursday, March 2

MS228

Quadrature Methods for Singular and Nearly Singular Integrals in Integral Equations - Part II of II

2:15 PM-3:55 PM

Room:209

For Part 1 see MS202

One of the main challenges for integral equation based numerical methods is the numerical integration of singular and nearly singular integrals. This minisymposium will focus on efforts to design accurate quadrature methods that can be efficiently applied for integrals over 3D surfaces.

Organizer: Anna-Karin Tornberg

KTH Royal Institute of Technology, Sweden

2:15-2:35 Computing Singular or Nearly Singular Integrals on Smooth Closed Surfaces

J. Thomas Beale, Duke University, USA; Wenjun Ying, Shanghai Jiao Tong University, China; Jason R. Wilson, Virginia Tech, USA

2:40-3:00 On the Solution of Elliptic Partial Differential Equations on Regions with Corners

Kirill Serkh, Yale University, USA

3:05-3:25 Generalized Gaussian Quadratures for Singular and Hypersingular Kernels

Zydrunas Gimbutas, National Institute of Standards and Technology, USA

3:30-3:50 High-Accuracy Discretization of Integral Operators on Smooth Surfaces

James Bremer, University of California, Davis, USA

Thursday, March 2

MS229

Advanced Computational Methods for Embedded Interfaces and Boundaries - Part I of II

2:15 PM-3:55 PM

Room:210

For Part 2 see MS256

Embedded/immersed boundary methods obviate the need for continual re-meshing in many applications involving rapid prototyping and design. A number of new methodologies have been recently developed, ranging from finite difference to finite element methods, in which remedies to some long standing problems regarding stability, robustness, accuracy, and flexibility have recently been introduced. This minisymposium attempts to bring together members of various scientific communities to present their most recent advances in this field. Applications include but are not confined to fluid and solid mechanics, fluid/structure interaction, multiphase flows, electromagnetics, radiation, etc.

Organizer: Guglielmo Scovazzi

Duke University, USA

Organizer: Alex Main

Duke University, USA

2:15-2:35 A Ghost-Fluid Method for Shock Hydrodynamics of Multi-Phase Flows

Xianyi Zeng, University of Texas at El Paso, USA; Kangan Li and Guglielmo Scovazzi, Duke University, USA

2:40-3:00 The Shifted Boundary Method for Embedded Domain Mechanics: A Variational Implementation Using the Nitsche Approach

Guglielmo Scovazzi, Alex Main, Ting Song, and Nabil Atallah, Duke University, USA

3:05-3:25 A Variational Shifted Boundary Method for CFD and Fluid/Structure Interaction Simulations

Alex Main, Ting Song, Nabil Atallah, and Guglielmo Scovazzi, Duke University, USA

3:30-3:50 A Shifted Boundary Method for Shallow Water Flows

Ting Song, Alex Main, and Guglielmo Scovazzi, Duke University, USA

Thursday, March 2

MS230

Advances in Nonstandard Finite Element Methods for Interface Problems - Part I of II

2:15 PM-3:55 PM

Room:211

For Part 2 see MS257

Real-world applications involving multiple materials or physics often lead to the so-caller interface problems. Solution to interface problems involves kinks, discontinuities, singularities, and other non-smooth features. In past decades, many nonstandard finite element methods (FEM) have been developed to solve interface problems efficiently, such as Generalized/Extended FEM, Nitche's FEM, Immersed FEM. This minisymposium will bring together experts in these fields to discuss recent advances in developing and analyzing nonstandard finite element methods for interface problems.

Organizer: Xu Zhang

Mississippi State University, USA

Organizer: Uday Banerjee

Syracuse University, USA

2:15-2:35 Solving an Inverse Interface Problem with a Fixed Mesh

Tao Lin, Virginia Tech, USA; Min Lin, Southwest University, China

2:40-3:00 Recent Advances in Embedded Finite Element Methods

John Dolbow, Duke University, USA

3:05-3:25 Gradient Recovery for Elliptic Interface Problem

Hailong Guo and *Xu Yang*, University of California, Santa Barbara, USA

3:30-3:50 On the Error Estimates of An Unfitted Nitsche Method Applied to Interface Problem

Manuel Sanchez-Uribe, University of Minnesota, USA; Erik Burman, University College London, United Kingdom; Johnny Guzman, Brown University, USA; Marcus Sarkis, Worcester Polytechnic Institute, USA, and Instituto de Matematica Pura e Aplicada (IMPA), Brazil

Thursday, March 2

MS231

Innovative Time Integrators for Large-Scale Complex Problems - Part I of II

2:15 PM-3:55 PM

Room:212

For Part 2 see MS258

Many complex systems in science and engineering require numerical solution of evolution equations that describe their dynamics over time. Many of these systems involve a wide spectrum of spatial and temporal scales, which makes numerical solution of the corresponding equations a difficult task. Over the past several decades many novel time integration techniques have been introduced to address these challenges. The goal of this minisymposium is to present some of the latest developments in numerical time integration. The minisymposium will connect numerical analysts working in time integration with practitioners and researchers from other fields of computational science and engineering.

Organizer: Vu Thai Luan

University of California, Merced, USA

Organizer: Mayya Tokman

University of California, Merced, USA

2:15-2:35 SUNDIALS Time Integrators and their Application

Carol S. Woodward, Lawrence Livermore National Laboratory, USA; Daniel R. Reynolds, Southern Methodist University, USA; David J. Gardner, Slaven Peles, Alan Hindmarsh, and L. Edward Banks, Lawrence Livermore National Laboratory, USA

2:40-3:00 Faster and More Accurate Pseudospectral DNS Through Adaptive High-Order Time Integration

David I. Ketcheson and Matteo Parsani, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Nathanael Schilling, Technische Universität München, Germany

continued in next column

3:05-3:25 Flexible and Accurate Multiphysics Time Integration with Arkode

Daniel R. Reynolds, Southern Methodist University, USA; David J. Gardner and Carol S. Woodward, Lawrence Livermore National Laboratory, USA; Jean Sexton, Southern Methodist University, USA

3:30-3:50 Domain Decomposition of Parabolic Equations - A Splitting Approach

Eskil Hansen, Lund University, Sweden

Thursday, March 2

MS232

Topology Optimization: Formulations, Methods and Applications - Part II of II

2:15 PM-3:30 PM

Room:213

For Part 1 see MS206

Topology optimization is a computational methodology for distributing two or more materials in a given design domain by minimizing a selected objective subject to physical constraints (e.g. compliance minimization subject to weight constraint). Initially applied to problems mainly in structural mechanics the methodology has been utilized in a number of other fields such as microelectromechanical systems, photonics, acoustics and fluid mechanics. Topology optimization is well accepted in industrial design processes where it can provide competitive designs in terms of cost, materials and functionality under a wide set of constraints. The methodology is typically implemented as a PDE constrained optimization problem which presents a number of mathematical challenges, including numerical methods for optimization, fast PDE solvers, and optimization formulations. Therefore, the minisymposium aims to explore these topics and present topology optimization approaches in a range of application spaces.

Organizer: Eric C. Cyr

Sandia National Laboratories, USA

Organizer: Boyan S. Lazarov

Technical University of Denmark, Denmark

2:15-2:35 Topology Optimization of Compact Wideband Coaxial-to-Waveguide Transitions with Minimum-Size Control

Martin Berggren, Emadeldeen Hassan, Linus Hagg, and Eddie Wadbro, Umeå University, Sweden

continued in next column

2:40-3:00 Adaptive Finite Element Method for Topology Optimization with Stress-Based Constraints

Miguel Salazar de Troya, Lawrence Livermore National Laboratory, USA; Daniel Tortorelli, University of Illinois at Urbana-Champaign, USA

3:05-3:25 Topology Optimization for Design of Coaxial Cables

Eric Cyr, Gregory J. von Winckel, Thomas Gardiner, Drew P. Kouri, and John Shadid, Sandia National Laboratories, USA

Thursday, March 2

MS233

Meshless, Particle, and Particle-Mesh Methods for PDEs - Part II of II

2:15 PM-3:55 PM

Room:214

For Part 1 see MS207

Due to their inherent scalability, meshless, particle-based and particle-mesh methods are becoming increasingly important with recent increases in available computing power. Meshless and particle-based methods provide adaptive solutions for problems with deforming interfaces, without the burden of generating boundary conforming meshes. Particle and particle-mesh methods become critically important as scientific and engineering applications move towards more resolved / first principles approaches. In addition to classical applications of particle methods for PDEs in electromagnetism and cosmology, new applications in climate, energy, and environmental areas are adopting particle and hybrid methods. We focus on recent developments using these methods to scalably solve PDEs with diverse applications to scientific and engineering problems. In particular, a spectrum of methods will be represented: Lagrangian particle methods for hydrodynamic problems, recent advances in smoothed particle hydrodynamics, staggered moving least squares, PIC methods for plasma physics problems, as well as topics from scattered data approximation theory. Research issues of particular interest include rigorous foundations of methods based on mathematical approximation theory, error analysis and convergence, improved kernels and high order methods, spatial and temporal adaptivity, and scalability on modern supercomputer architectures.

Organizer: Nathaniel Trask

Sandia National Laboratories, USA

continued on next page

2:15-2:35 Meshless Approximation Using RBF-Partition of Unity Method with Applications to the Reconstruction of Basins of Attraction in Dynamical Systems

Alessandra De Rossi, Roberto Cavoretto, and Emma Perracchione, Università di Torino, Italy

2:40-3:00 Radial Basis Functions

Grady B. Wright, Boise State University, USA

3:05-3:25 High-Order Radial Basis Function Finite Difference Methods for the Meshfree Solution of PDEs on Time-Varying Irregular Domains

Varun Shankar and Aaron L. Fogelson, University of Utah, USA

3:30-3:50 Numerical Study of Space-Time RBF Method for PDEs

Alfa Heryudono, University of Massachusetts, Dartmouth, USA

Thursday, March 2

MS234

Evolution of Co-Design and Scientific HPC Applications - Part II of II

2:15 PM-3:30 PM

Room:215

For Part 1 see MS208

Modernizing scientific codes to run performantly on multiple emerging architectures is a task of great complexity and challenge for computational scientists today. It is typical the set of performance necessary optimizations for a code on a given platform will be distinct from those for another. To ameliorate this difficulty, we turn to abstraction layers and alternative programming models. This minisymposium will present the integrations of small-scale experiments into production level codes, programming models and runtimes which support them, and other research towards next-generation scientific HPC applications.

Organizer: Geoff Womeldorff

Los Alamos National Laboratory, USA

Organizer: Ian Karlin

Lawrence Livermore National Laboratory, USA

2:15-2:35 The Flexible Computational Science Infrastructure (flecsi) Project: Interfaces for Multi-Physics Applications Development

Ben Bergen, Marc Charest, Irina Demeshko, Nick Moss, and Joshua Payne, Los Alamos National Laboratory, USA

2:40-3:00 (Re-)Designing Iterative Solvers for Task-Based Runtime Systems

Steven Dalton, NVIDIA, USA

3:05-3:25 Stapl, Spatial Decomposition, and Problem Space Representations for Compact Binary Mergers

Glen Hordemann, Texas A&M University, USA; Nicolas de Brye, University of Valencia, Spain; Daniel George, University of Illinois at Urbana-Champaign, USA; Hyun Lim, Brigham Young University, USA; Julien Loiseau, Universite de Reims, France; Jonah Miller, Perimeter Institute For Theoretical Physics, Canada; Jonathan Sharman, Rice University, USA

Thursday, March 2

MS235

Coarse-Graining, Stochastic Parametrizations and the Mori-Zwanzig Formulation - Part II of II

2:15 PM-3:55 PM

Room:216

For Part 1 see MS209

Microscopic simulations based on interacting particles are becoming increasingly prevalent in the modeling of complex systems such as those in material science, biology and soft matter physics. One of the main objectives of such simulations is understand large-scale effects based on microscopic first principles. The computational cost of particle-based simulations depends critically on the number of particles and the interaction potentials, and can require hundred of thousands of computer cores and significant computing time and data processing to be successfully completed. This motivates the use of coarse-graining techniques such as the Mori-Zwanzig formulation to compute macroscopic/mesoscopic observables at a reasonable computational cost. This minisymposium invites contributions that showcase the potential and effectiveness of coarse-graining techniques in applied sciences, including particle models and multi-scale stochastic dynamical systems.

Organizer: Jason Dominy

University of California, Santa Cruz, USA

2:15-2:35 Nonlocal Models for Nanoscale Heat Conduction

Xiantao Li, Pennsylvania State University, USA

2:40-3:00 Dynamic Sub-Grid Scalthe Mori-Zwanzig Formalisme Models for Large Eddy Simulations Based on

Eric Parish, University of Michigan, USA; Karthik Duraisamy, University of Michigan, Ann Arbor, USA

continued on next page

Thursday, March 2

MS235

Coarse-Graining, Stochastic Parametrizations and the Mori-Zwanzig Formulation - Part II of II

2:15 PM-3:55 PM

continued

3:05-3:25 Efficient Exploration of the Conformational Space of Proteins Using the Concurrent Adaptive Sampling Algorithm

Surl-Hee Ahn, Stanford University, USA; Jay Grate, Pacific Northwest National Laboratory, USA; Eric F. Darve, Stanford University, USA

3:30-3:50 Brownian Dynamics Approximation to Generalized Langevin Equations

Lina Ma, Xiantao Li, and Chun Liu, Pennsylvania State University, USA

Thursday, March 2

MS236

Tensor Decompositions: Applications and Efficient Algorithms - Part II of II

2:15 PM-3:55 PM

Room:217

For Part 1 see MS210

Tensors, or multidimensional arrays, are a natural way to represent high-dimensional data arising in a multitude of applications. Tensor decompositions, such as the CANDECOMP/PARAFAC and Tucker models, help to identify latent structure, achieve data compression, and enable other tools of data analysis. This minisymposium identifies pressing applications for multidimensional data analysis as well as efficient algorithms for computing various tensor decompositions.

Organizer: Grey Ballard

Wake Forest University, USA

Organizer: Tamara G. Kolda

Sandia National Laboratories, USA

Organizer: Bora Ucar

LIP-ENS Lyon, France

2:15-2:35 Tensor Decompositions for Bernoulli Data

Tamara G. Kolda and Cliff Anderson-Bergman, Sandia National Laboratories, USA

2:40-3:00 An Exploration of Optimization Algorithms for High Performance Tensor Completion

Shaden Smith, University of Minnesota, USA; Jongsoo Park, Intel Corporation, USA; George Karypis, University of Minnesota and Army HPC Research Center, USA

3:05-3:25 Performing Successive Tensor-Times-Matrix and -Vector Multiplies using Dimension Trees

Oguz Kaya, Inria and ENS Lyon, France; Bora Ucar, LIP-ENS Lyon, France

3:30-3:50 Efficient Parallel Software for Tucker Decompositions of Dense Tensors

Alicia Klinvex, Sandia National Laboratories, USA; Grey Ballard, Wake Forest University, USA; Tamara G. Kolda, Sandia National Laboratories, USA

Thursday, March 2

MS237

Algorithmic Revolution in Post Moore's Era : Auto-Tuning and Accuracy Assurance - Part II of II

2:15 PM-3:55 PM

Room:218

For Part 1 see MS211

It is expected that by the end of 2020 no gains in FLOPS counting will be achieved with a constant power budget due to physical limitations in device miniaturization. This inflection point, referred to as "Post Moore's Era", is already leading researchers to consider that the ability to memory access (BYTES) is becoming more relevant than a growing FLOPS. Hence, an algorithmic revolution, from FLOPS to BYTES, will be necessary for efficient numerical computations. We believe that auto-tuning (AT) technologies will be built upon it is proven success path, and have the ability of providing optimized, high performance implementations of specific computations for architectures of the Post Moore's Era. It is expected that these architectures will enable the solution of problems with unprecedented levels of details, implying very large problems, which in turn raises concerns about the accuracy of the computations. Usually, codes that perform floating point sums of distributed data cannot expect the results to be reproducible. This is likely to be exacerbated in the Post Moore's Era; thus an increasing interest about how to address nonreproducibility in large applications. This minisymposium will discuss technologies for AT and its interplay with accuracy assurance towards the Post Moore's Era.

Organizer: Toshiyuki Imamura

RIKEN Advanced Institute for Computational Science, Japan

Organizer: Osni A. Marques

Lawrence Berkeley National Laboratory, USA

continued on next page

Organizer: Takahiro Katagiri
Nagoya University, Japan

2:15-2:35 Performance of the Quadruple Precision Eigensolver Library QPEigenK on Supercomputer Systems
Yusuke Hirota, RIKEN Advanced Institute for Computational Science, Japan; Susumu Yamada, Japan Atomic Energy Agency, Japan; Toshiyuki Imamura, RIKEN Advanced Institute for Computational Science, Japan; Narimasa Sasa, Yasuhiro Idomura, Takuya Ina, and Masahiko Machida, Japan Atomic Energy Agency, Japan

2:40-3:00 Reproducibility of Linear Algebra Operations
Roman Iakymchuk, KTH Royal Institute of Technology, Sweden; Stef Graillat, University Pierre and Marie Curie (UPMC), France; David Defour, University of Perpignan, France; Sylvain Collange, Inria Rennes, France; Enrique S. Quintana-Orti, Universidad Jaume I, Spain; Erwin Laure, KTH Royal Institute of Technology, Sweden

3:05-3:25 Faithful Rounding for Matrix Multiplication
Katsuhisa Ozaki, Shibaura Institute of Technology, Japan; Takeshi Ogita, Tokyo Woman's Christian University, Japan

3:30-3:50 Reproducible Parallel Simulations in {HPC}
Chemseddine Chohra, *Philippe Langlois*, Rafife Nheili, and David Parello, University of Perpignan, France

Thursday, March 2

MS238

Recent Developments in Linear System Solvers Based on Low-rank Approximation Techniques - Part II of II

2:15 PM-3:55 PM

Room:219

For Part 1 see MS212
The primary goal of this minisymposium is to discuss recent developments in linear system solvers based on low-rank approximation techniques. Low-rank approximation techniques have drawn much attention in recent years and led to much progress in developing more efficient methods for solving large scale linear systems. These techniques resulted in fast direct solvers based on (nearly) linear time matrix factorizations or inversions and robust preconditioners for indefinite and ill-conditioned systems. All the 8 presentations in this minisymposium have shown relevant and of great importance to this topic. The applications ranges from PDEs, integral equations, machine learning applications, etc.

Organizer: Yuanzhe Xi
University of Minnesota, USA

Organizer: Ruipeng Li
Lawrence Livermore National Laboratory, USA

2:15-2:35 Fast Construction of Some Hierarchical Rank Structured Matrices with Nested Bases
Difeng Cai, Purdue University, USA; Yuanzhe Xi and Yousef Saad, University of Minnesota, USA; Edmond Chow, Georgia Institute of Technology, USA

2:40-3:00 Interconnected Hierarchical Structures for Solving Non-Coercive Elliptic PDEs
Xiao Liu, Rice University, USA; Maarten de Hoop and Jianlin Xia, Purdue University, USA

3:05-3:25 Randomized QR with Column Pivoting
Jed Duersch, University of California, Berkeley, USA

3:30-3:50 Reliable Randomized Spectrum Revealing Matrix Factorizations
Jianwei Xiao and Ming Gu, University of California, Berkeley, USA

Thursday, March 2

MS239

Science and Engineering Applications of Derivative-Free Optimization - Part II of II

2:15 PM-3:55 PM

Room:220

For Part 1 see MS213
Numerical optimization arises throughout computational science and engineering, from design optimization and optimal control to model calibration and data assimilation. This minisymposium concerns settings where some derivatives of the objective function and/or constraints are unavailable or otherwise unreliable. The talks will address a diverse set of challenges that arise in different applications and will highlight how these challenges pose problem for classical optimization methods. Presented will be recent algorithmic and computational advances that enable solution of difficult science and engineering problems that were previously out of reach.

Organizer: Stefan Wild
Argonne National Laboratory, USA

2:15-2:35 Efficient Sampling Allocation Using Multi-Fidelity Information in Simulation Optimization
Yijie Peng, George Mason University, USA and Fudan University, China; *Jie Xu* and Chun-Hung Chen, George Mason University, USA; Loo Hay Lee, National University of Singapore, Singapore

2:40-3:00 Multi-Fidelity Surrogate Modeling of Expensive Cosmology Functions
Juliane Mueller, Zarija Lukic, and Dmitriy Morozov, Lawrence Berkeley National Laboratory, USA

3:05-3:25 Global Optimization with Native Space Semi-Norm Bounds
David Eriksson, David Bindel, and Christine A. Shoemaker, Cornell University, USA

3:30-3:50 Tuning the Global Optimization Solver BARON using Derivative-Free Optimization Algorithms
Nikolaos Ploskas, Jianfeng Liu, and Nikolaos Sahinidis, Carnegie Mellon University, USA

Thursday, March 2

MS240

Parallel Implementations of Hierarchical Matrix-Based Algorithms - Part II of II

2:15 PM-3:55 PM

Room:Crystal AF - 1st Fl

For Part 1 see MS214

In the last two decades, there have been substantial theoretical and practical advances in the area of fast direct solvers, often relying on hierarchical low-rank approximations in its different data-sparse formats. Leveraging these contributions is most needed today as computer hardware changes rapidly and the need to solve relevant problems efficiently is ever present. This minisymposium focuses on the synergies between theory and practical implementations of a variety of algorithms that by exploiting a hierarchy of low-rank approximations deliver optimal complexity scalable solvers for relevant problems in science and engineering.

Organizer: Pieter Ghysels

Lawrence Berkeley National Laboratory, USA

Organizer: Gustavo Chavez

King Abdullah University of Science & Technology (KAUST), Saudi Arabia

Organizer: David E. Keyes

King Abdullah University of Science & Technology (KAUST), Saudi Arabia

2:15-2:35 Accelerating Parallel Optimization Methods with Hierarchical Matrix Computations

James Vogel and Jianlin Xia, Purdue University, USA

2:40-3:00 Sparse Supernodal Solver Using Hierarchical Compression over Runtime System

Gregoire Pichon, Université de Bordeaux, Inria, LaBRI, France; Eric F. Darve, Stanford University, USA; Mathieu Faverge and Pierre Ramet, Université de Bordeaux, Inria, LaBRI, France; Jean Roman, Inria, France

continued in next column

3:05-3:25 Hierarchical Matrix Operations on GPUs

Wajih Halim Boukaram, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; G*eorge M Turkiyyah*, American University of Beirut, Lebanon; David E. Keyes and Hatem Ltaief, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

3:30-3:50 Breaking the O(N) Barrier for Solving the High-Frequency Helmholtz Equation

Russell Hewett, Total E&P, USA; Leonardo Zepeda-Nunez, University of California, Irvine, USA; Adrien Scheuer, Université Catholique de Louvain, Belgium; Laurent Demanet, Massachusetts Institute of Technology, USA

Thursday, March 2

MS241

New Approaches to Complex Coupled Multiscale Systems - Part II of II

2:15 PM-3:55 PM

Room:Crystal CD - 1st Fl

For Part 1 see MS215

As the fidelity of computational algorithms increases, and the computational resources (hardware and software simulation systems) become more available, computational and applied mathematics can now simulate a variety of complex coupled phenomena with multiple scales which were unfeasible a decade ago. However, the complexity of real world and the availability of data poses new challenges in order to move beyond the proof-of-concept realizations and closer to the goal of describing and managing real-life applications with meaningful objectives. In this minisymposium the presentations will describe novel modeling and algorithmic approaches which can work with, and interpret real data.

Organizer: Malgorzata Peszynska

Oregon State University, USA

2:15-2:35 Consolidation of a Sedimentary Basin

Ralph E. Showalter and Dwight Holland, Oregon State University, USA

2:40-3:00 Virtual Farming: Combining Knowledge to Enhance Decision-Making in Agricultural Regions

Eleanor Jenkins, Clemson University, USA; Kathleen Kavanagh, Clarkson University, USA

3:05-3:25 Multiscale Integration of Blood Flow Mechanics and Neural Signaling to Model Retinal Microcirculation

Riccardo Sacco, Aurelio G. Mauri, and Alessandra Cardani, Politecnico di Milano, Italy; Giovanna Guidoboni, Indiana University - Purdue University Indianapolis, USA; Alon Harris, Indiana University School of Medicine, USA

3:30-3:50 Mixed Methods for Two-Phase Darcy-Stokes Mixtures of Partially Melted Materials with Regions of Zero Porosity

Todd Arbogast, Marc A. Hesse, and Abraham Taicher, University of Texas at Austin, USA

Thursday, March 2

MS242

Flow-Induced Shaping Processes: Erosion, Dissolution, Ablation, and Phase Change - Part II of II

2:15 PM-3:55 PM

Room:301

For Part 1 see MS216

All around us, solid material is shaped, transported, and obliterated by flowing fluids, from soil and sediment on Earth's surface to plaque within human arteries. These material-removal processes - including erosion, dissolution, ablation, and melting - will be the focus of this special session. Particular emphasis will be placed on geophysical examples and on viewing these processes from the moving-boundary-problem perspective. The session will feature theoretical modeling and numerical simulations, as well as laboratory experiments and field measurements. It will bring together scientists and mathematicians from a range of backgrounds.

Organizer: Matthew N. Moore

Florida State University, USA

Organizer: Bryan D. Quaife

Florida State University, USA

2:15-2:35 Interfacial Dynamics of Dissolving Objects from Discrete and Continuum Perspectives

Chris H. Rycroft and Yuexia Lin, Harvard University, USA

2:40-3:00 Sculpting of a Dissolving Body

Jinzi Mac Huang, New York University, USA; Megan Davies Wykes, Courant Institute of Mathematical Sciences, New York University, USA; Nick Moore, Florida State University, USA; Leif Ristroph, Courant Institute of Mathematical Sciences, New York University, USA

3:05-3:25 Do Dissolving Objects Converge to a Universal Shape?

Elias Nakouzi, Florida State University, USA

3:30-3:50 Severe Erosion of a Cylinder Within the Subcritical Reynolds Range

James N. Hewett and Mathieu Sellier, University of Canterbury, New Zealand

Thursday, March 2

MS243

Theoretical and Computational Advancements in Ice Sheet Modeling - Part II of II

2:15 PM-3:55 PM

Room:302

For Part 1 see MS217

Accurately modeling the dynamics of large ice sheets is essential for projections of sea level rise in the 21st century, but faces many mathematical challenges. Ongoing research includes the development of accurate and tractable models for ice sheet dynamics (e.g., models featuring more physically correct temperature effects, boundary conditions, and/or domain movement, etc.), coupling between ice dynamics and other climate components, (e.g., atmosphere, ocean, etc.) necessary for global climate simulations, and data assimilation, to calibrate parameters and/or initial/boundary conditions. This minisymposium addresses advancements in the development of stand-alone and coupled land-ice models, as well as computational strategies to tackle the resulting discrete problems.

Organizer: Luca Bertagna

Florida State University, USA

Organizer: Mauro Perego

Sandia National Laboratories, USA

Organizer: Irina K. Tezaur

Sandia National Laboratories, USA

Organizer: Daniel Martin

Lawrence Berkeley National Laboratory, USA

continued in next column

2:15-2:35 Joint Model and Parameter Dimension Reduction for Bayesian Inversion Applied to an Ice Sheet Problem

Noemi Petra, University of California, Merced, USA; Tiangang Cui, Monash University, Australia; Omar Ghattas, University of Texas at Austin, USA; Youssef M. Marzouk, Benjamin Peherstorfer, and Karen E. Willcox, Massachusetts Institute of Technology, USA

2:40-3:00 A Three-Dimensional, Implicit, Thermo-Mechanical Computational Model for Polythermal Ice

Alessandro Barone, Emory University, USA; *Mauro Perego*, Sandia National Laboratories, USA

3:05-3:25 PISM-FEvoR: A Multi-Scale Ice Flow Model Incorporating Fabric Evolution with Recrystallization

Joseph H. Kennedy, Oak Ridge National Laboratory, USA; Constantine Khroulev, University of Alaska, Fairbanks, USA; Florian Ziemen, Max Planck Insitute for Meteorology, Germany; Erin Pettit, University of Alaska, Fairbanks, USA

3:30-3:50 Demonstration of Unstructured Mesh Adaptation for Ice Sheet Modeling Applications

Mauro Perego, Sandia National Laboratories, USA; Cameron Smith and Dan A. Ibanez, Rensselaer Polytechnic Institute, USA; *Glen Hansen* and Irina K. Tezaur, Sandia National Laboratories, USA; Mark S. Shephard, Rensselaer Polytechnic Institute, USA

Thursday, March 2

MS244

Advances in Methods with the Summation-by-Parts Property - Part II of II

2:15 PM-3:55 PM

Room:303

For Part 1 see MS218

As we move towards an era of exascale HPC, flexible and robust algorithms will be necessary to take advantage of increasingly complex and failure prone computational resources. In this minisymposium, the focus is on methods having the summation-by-parts (SBP) property, which are advantageous as they lead to high-order methods that are provably conservative and stable. In particular, the interest is in recent advancements leading to improved efficiency, flexibility, and robustness. Topics that will be covered include: Stable and conservative coupling procedures for non- conforming elements and mesh adaptation; Nonlinearly stable algorithms; Discretization of split forms.

Organizer: David C. Del Rey Fernandez

University of Toronto Institute for Aerospace Studies, Canada

Organizer: Jason E. Hicken

Rensselaer Polytechnic Institute, USA

Organizer: Andrew R. Winters

University of Cologne, Germany

2:15-2:35 Toward Entropy-Stable Gas-Dynamics Simulations Using Tetrahedral SBP Elements

Jared Crean and Jason E. Hicken, Rensselaer Polytechnic Institute, USA

2:40-3:00 BR1 is not Unstable for the Compressible Navier-Stokes Equations

David A. Kopriva, Florida State University, USA; Gregor Gassner and Andrew R. Winters, University of Cologne, Germany

continued in next column

3:05-3:25 Efficiency Assessment of Split Form Nodal Discontinuous Galerkin Schemes for the Compressible Navier-Stokes Equations

Andrew R. Winters, University of Cologne, Germany; Florian Hindenlang, ; Gregor Gassner, University of Cologne, Germany

3:30-3:50 Fourth-Order Entropy Stable Non-Oscillatory Spectral Collocation Schemes

Mark H. Carpenter, NASA Langley Research Center, USA

Thursday, March 2

MS245

Multiscale Models and Algorithms for Materials Science - Part II of II

2:15 PM-3:55 PM

Room:304

For Part 1 see MS219

Multiscale material models aim to capture highly nonlinear phenomenon arising from molecular-level behavior and its interaction with larger scale materials properties, while vastly reducing the computational costs compared to direct simulation. This minisymposium brings together contributions to the development and analysis of algorithms handling a wide range of problems such as defect-laden materials, non-local behavior, finite temperature effects, and multiscale dynamical interactions.

Organizer: Matthew Dobson

University of Massachusetts, Amherst, USA

Organizer: Xingjie Li

University of North Carolina, Charlotte, USA

2:15-2:35 Bridging Time and Length-Scales in Dislocation Dynamics

Thomas Hudson, University of Warwick, United Kingdom

2:40-3:00 Large-Scale Real-Space Electronic Structure Calculations

Vikram Gavini, University of Michigan, USA

3:05-3:25 Data-Driven Parameterization of Generalized Langevin Equation

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

3:30-3:50 Propagating Fluctuations Across Atomistic and Mesoscopic Simulations

Xin Bian, Technische Universität München, Germany; Weinan E, Princeton University, USA; George E. Karniadakis, Brown University, USA

Thursday, March 2

MS246

Adaptive Methods for Uncertainty Quantification and Error Estimation - Part II of II

2:15 PM-3:55 PM

Room:305

For Part 1 see MS220

A common goal in scientific computation is to quantify uncertainties and/or estimate errors of specific prediction or input quantities of interest. As computational models become more complex, the dimension of the input/output spaces increase, or the UQ/error estimation method becomes more sophisticated, some form of adaptivity must be employed to circumvent various computational issues arising from finite computational budgets.

Organizer: Jehanzeb H. Chaudhry

University of New Mexico, USA

Organizer: Troy Butler

University of Colorado, Denver, USA

2:15-2:35 Uncertainty Quantification for Approximate P-Quantiles for Physical Models with Stochastic Inputs

Don Estep, Colorado State University, USA; Daniel Elfverson, Umeå University, Sweden; Fredrik Hellman, Uppsala University, Sweden; Axel Malqvist, Chalmers University of Technology, Sweden

2:40-3:00 Combined Uncertainty and A Posteriori Bounds for CFD Calculations

Timothy J. Barth, NASA Ames Research Center, USA

3:05-3:25 Output-Based Adaptation for Chaotic Flow Simulations

Krzysztof Fidkowski and Yukiko Shimizu, University of Michigan, USA

3:30-3:50 Goal-Based Adaptive Control for Uncertainties Dominated Compressible Flows

Anca Belme, Université Paris VI, France

Thursday, March 2

MS247

Hydrodynamics at Small Scales: Passive and Active Fluctuations - Part II of II

2:15 PM-3:55 PM

Room:221

For Part 1 see MS221

With the increased interest in nano- and micro-fluidics, as well as biological systems, it has become necessary to develop tools for hydrodynamic calculations at microscopic and mesoscopic scales. This minisymposium will focus on advances in multiscale numerical methods for simulating flows at mesoscopic scales. Of particular interest will be fluctuating hydrodynamics of complex fluids such as reactive mixtures, colloidal passive and active suspensions, and multi-phase fluids. Issues to be discussed will include the inclusion of thermal fluctuations in analytical and computational models, as well as applications in the physical sciences, biology, and engineering.

Organizer: Aleksandar Donev

Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Andrew Nonaka

Lawrence Berkeley National Laboratory, USA

2:15-2:35 Collective Colloid Diffusion Under Soft 2D Confinement

Rafael Delgado Buscalioni, Universidad Autonoma de Madrid, Spain

2:40-3:00 A Rigid Multiblob Algorithm for Confined Brownian Suspensions

Brennan Sprinkle, Northwestern University, USA; Florencio Balboa Usabiaga, Universidad Autonoma de Madrid, Spain; Neelesh Patankar, Northwestern University, USA; Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA

3:05-3:25 Brownian Dynamics for a Confined Suspension of Microrollers

Florencio Balboa Usabiaga, Blaise Delmotte, and Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA

continued in next column

3:30-3:50 A Fluctuating Boundary Integral Method for Brownian Suspensions

Yuanxun Bill Bao and Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA; Eric Keaveny, Imperial College London, United Kingdom; Leslie Greengard, Courant Institute of Mathematical Sciences, New York University, USA; Manas N. Rachh, Yale University, USA

Thursday, March 2

CP17

Life Sciences - Part I of II

2:15 PM-3:55 PM

Room:223

For Part 2 see CP19

2:15-2:25 Models for Principled Characterization of Dynamic, Spatially Embedded, Multiscale Networks

Richard Betzel, University of Pennsylvania, USA

2:27-2:37 Numerical Simulation of a Nonlocal Variational Problem

Chong Wang, Xiaofeng Ren, and Yanxiang Zhao, George Washington University, USA

2:39-2:49 Educational Modules on HPC Bioinformatics Algorithms

Angela B. Shiflet, George W. Shiflet, and Daniel Couch, Wofford College, USA; Pietro Guzzi and Mario Cannataro, Università degli Studi di Catanzaro "Magna Graecia", Italy

2:51-3:01 Mathematical Modeling and Numerical Simulation of Drug Delivery in the Coronary Arterial Wall Using Drug Eluting Stent

Jahed Naghipoor, Bauhaus-Universität Weimar, Germany; Jose Augusto Ferreira and Lino Goncalves, University of Coimbra, Portugal; Timon Rabczuk, Bauhaus-Universität Weimar, Germany; Paula de Oliveria, University of Coimbra, Portugal

3:03-3:13 Influence of Scaffold Permeability on Tissue Growth in a Perfusion Bioreactor

Daniel Fong, United States Merchant Marine Academy, USA; Linda Cummings and Jeff Pohlmeyer, New Jersey Institute of Technology, USA

3:15-3:25 Comparison of Different Algorithms for Biomolecule Simulations

Weishan Deng, Xiaohe Zhufu, and Jin Xu, Chinese Academy of Sciences, China

Thursday, March 2

CP18

Numerical PDEs - Part VI of VI

2:15 PM-3:55 PM

Room:224

For Part 5 see CP16

Chair: Jennifer Proft, University of Texas at Austin, USA

2:15-2:25 Influence of Storm Characteristics on Hurricane Surge

Jennifer Proft and Clint Dawson, University of Texas at Austin, USA

2:27-2:37 Fluctuating Hydrodynamic Methods for Manifolds: Particle Dynamics Within Curved Fluid Interfaced and Membranes

Ben J. Gross and Paul Atzberger, University of California, Santa Barbara, USA

2:39-2:49 Mathematical Modeling and Analysis of a Type-3 DFIG/DFAG Wind Turbine Dynamics: Numerical, Analytical, and Simulation Results

Sameh Eisa, William Stone, and Kevin Wedeward, New Mexico Institute of Mining and Technology, USA

2:51-3:01 Numerical Methods for Stochastic Differential Equations with Highly Nonlinear Coefficients

Zhongqiang Zhang, Worcester Polytechnic Institute, USA

3:03-3:13 Approximating Optimal Local Subspaces for Localized Model Order Reduction By Random Sampling

Kathrin Smetana, *Kathrin Smetana*, and Andreas Buhr, Universität Münster, Germany

3:15-3:25 Optimal Parametric Model Reduction in H2-L2 Norm

Alexander R. Grimm, Serkan Gugercin, and Christopher A. Beattie, Virginia Tech, USA

Coffee Break

3:55 PM-4:25 PM

Room:Foyer - 2nd Fl

Thursday, March 2

MS120

Space-Time Multigrid Methods

4:25 PM-6:05 PM

Room:304

The need for parallel-in-time algorithms is being driven by the rapid change in computer architectures towards systems with more, but not faster, processors. Future speedups will come through making use of this greater concurrency, not faster clock-speeds, which are stagnant. Overall, this leads to the sequential time integration bottleneck, because classic sequential time stepping scales neither strongly nor weakly. The bottleneck can only be avoided by exploiting parallelism in the time dimension. While a large variety of algorithms exists for parallel-in-time integration, one of the most prominent and flexible approaches is the application of space-time multigrid methods. Applying multigrid to the time dimension is attractive for the same reasons that multigrid in space is attractive: Full multilevel solvers like multigrid exhibit optimal algorithmic scaling and optimal parallel communication behavior. This minisymposium thus highlights this approach, focusing on the theory and application of different algorithms in this rapidly growing field of research.

Organizer: Matthias Bolten

Universität Kassel, Germany

Organizer: Jacob B. Schroder

Lawrence Livermore National Laboratory, USA

4:25-4:45 PFASST as a Space-Time Multigrid Method

Matthias Bolten, Universität Kassel, Germany; Dieter Moser and Robert Speck, Jülich Supercomputing Centre, Germany

4:50-5:10 Multigrid Reduction in Time with Full Space-Time Adaptivity

Ben O'Neill, University of Colorado Boulder, USA

5:15-5:35 MGRIT for Power-Grid Systems and BDF-K Methods

Matthieu B. Lecouvez, Lawrence Livermore National Laboratory, USA

5:40-6:00 Space-Time Multigrid Methods for Parabolic Problems

Martin Neumueller, Johannes Kepler Universität, Linz, Austria

Thursday, March 2

MS221

Hydrodynamics at Small Scales: Passive and Active Fluctuations - Part I of II

4:25 PM-6:05 PM

Room:305

For Part 2 see MS247

With the increased interest in nano- and micro-fluidics, as well as biological systems, it has become necessary to develop tools for hydrodynamic calculations at microscopic and mesoscopic scales. This minisymposium will focus on advances in multiscale numerical methods for simulating flows at mesoscopic scales. Of particular interest will be fluctuating hydrodynamics of complex fluids such as reactive mixtures, colloidal passive and active suspensions, and multi-phase fluids. Issues to be discussed will include the inclusion of thermal fluctuations in analytical and computational models, as well as applications in the physical sciences, biology, and engineering.

Organizer: Aleksandar Donev

Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Andrew Nonaka

Lawrence Berkeley National Laboratory, USA

4:25-4:45 Fluctuating Hydrodynamics of Reaction-Diffusion Systems

Changho Kim and *Andrew Nonaka*, Lawrence Berkeley National Laboratory, USA; Alejandro Garcia, San Jose State University, USA; John B. Bell, Lawrence Berkeley National Laboratory, USA; Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA

4:50-5:10 Low Mach Number Fluctuating Hydrodynamics for Electrolytes

Jean-Philippe M. Peraud and Andrew Nonaka, Lawrence Berkeley National Laboratory, USA; Anuj Chaudhri, Lawrence Livermore National Laboratory, USA; John B. Bell, Lawrence Berkeley National Laboratory, USA; Aleksandar Donev, Courant Institute of Mathematical Sciences, New York University, USA; Alejandro Garcia, San Jose State University, USA

5:15-5:35 A Finite Element Formulation of Fluctuating Hydrodynamics for Fluids Filled with Rigid Particles Using Boundary Fitted Meshes

Marco De Corato, Imperial College London, United Kingdom; Johan Slot and Markus Hutter, Technische Universiteit Eindhoven, The Netherlands; Gaetano D'Avino and Pier Luca Maffettone, University of Naples Federico II, Italy; Martien Hulsen, Technische Universiteit Eindhoven, The Netherlands

5:40-6:00 DSMC simulations of Brownian Motion of a Small Particle in Rarefied Gas

Sudarshan Tiwari and Axel Klar, Technische Universität Kaiserslautern, Germany; Steffen Hardt, Technische Universität Darmstadt, Germany; Samir Shrestha, Kathmandu University, Nepal; Tobias Baier, Technische Universität Darmstadt, Germany

continued in next column

Thursday, March 2

MS248

Computational Plasma Physics

4:25 PM-6:05 PM

Room:Grand Ballroom - 2nd Fl

Accurately and efficiently simulating the dynamics of plasma is important in a wide range of applications including astrophysics, space weather, confined fusion, particle accelerators, and semiconductor manufacturing. The simulation of plasma remains a challenging problem due to the great range of temporal and spatial scales inherent in plasma phenomena. This minisymposium addresses recent advances in numerical methods for fluid and kinetic models of plasmas.

Organizer: Andrew Chrislieb

Michigan State University, USA

Organizer: James A. Rossmanith

Iowa State University, USA

4:25-4:45 Stabilization of Numerical Interchange in Spectral-Element Magnetohydrodynamics

Carl Sovinec, University of Wisconsin, Madison, USA

4:50-5:10 Exact Preservation of Zero Velocity Divergence in a High-Order, Mapped-Grid, Finite-Volume Discretization of a Gyrokinetic System

Milo Dorr, Lawrence Livermore National Laboratory, USA; Phillip Colella, Lawrence Berkeley National Laboratory, USA; Mikhail Dorf, Debojyoti Ghosh, and Jeffrey A. Hittinger, Lawrence Livermore National Laboratory, USA

5:15-5:35 Implementation of Implicit-Explicit Time Integration for the Kinetic Modeling of Tokamak Plasma Edge

Debojyoti Ghosh, Milo Dorr, Mikhail Dorf, and Jeffrey A. Hittinger, Lawrence Livermore National Laboratory, USA

5:40-6:00 Astrophysical Plasmas at the Exascale: Challenges and Opportunities

Brian O'Shea, Michigan State University, USA

Thursday, March 2

MS249

Compressive Sampling Methods In High-Dimensional Stochastic and Parametric Approximations - Part II of II

4:25 PM-6:05 PM

Room:Ballroom D - 2nd Fl

For Part 1 see MS196

The development of scalable numerical methods for the solution of problems with high-dimensional stochastic or parametric inputs has been a subject of active research in computational sciences and engineering. This is motivated by the need to mitigate the difficulties associated with the rapid growth of computational complexity in the simulation of physical systems where accurate specification of governing equations entails a large number of parameters or stochastic inputs. One such approaches, known as compressive sampling, exploits the sparsity of the quantities of interest (QoI) — in a multivariate basis of inputs — by employing appropriate optimization/regularization techniques. In particular, when sufficiently sparse, the QoI may be accurately computed from a number of its random realizations that depends linearly on the sparsity, as opposed to the cardinality of the basis. This minisymposium presents state-of-the-art in compressive sampling developments for various aspects of high-dimensional computation, including analysis, algorithms, implementation, and applications.

Organizer: Dongbin Xiu
University of Utah, USA

Organizer: Alireza Doostan
University of Colorado Boulder, USA

4:25-4:45 Experimental Design In Sparse Polynomial Chaos Expansions

Alireza Doostan, University of Colorado Boulder, USA; Paul M. Diaz, Colorado School of Mines, USA; Paul Diaz, University of Colorado Boulder, USA

4:50-5:10 Polynomial Approximation Using Compressive Sampling and the Spectral Distribution

Akil Narayan, University of Utah, USA

5:15-5:35 Enhancing Sparsity of Generalized Polynomial Chaos Expansions

Xiu Yang, Pacific Northwest National Laboratory, USA; Xiaoliang Wan, Louisiana State University, USA; Lin Lin, University of California, Berkeley and Lawrence Berkeley National Laboratory, USA; Nathan Baker, Pacific Northwest National Laboratory, USA

5:40-6:00 Robust Compressive Sensing with Application to Multifidelity Analysis of Complex Turbulent Flows

Xun Huan, Cosmin Safta, Khachik Sargsyan, Michael S. Eldred, Zachary Vane, Guilhem Lacaze, Joseph C. Oefelein, and Habib N. Najm, Sandia National Laboratories, USA

continued in next column

Thursday, March 2

MS250

Nonlocal Models in Computational Science and Engineering - Part III of III

4:25 PM-6:05 PM

Room:202

For Part 2 see MS223

Nonlocal models provide a new framework to overcome limitations and challenges present in classical PDE-based models. For instance, peridynamics, a nonlocal extension of classical continuum mechanics, admits discontinuous solutions and naturally describes material failure and damage. Similarly, nonlocal and fractional diffusion models can represent anomalous diffusion and heat transfer. Furthermore, nonlocal models introduce length scales, which can be used for multiscale modeling. Recent years have witnessed a tremendous advance in modeling, mathematical analysis, and computational practice for nonlocal problems. This minisymposium focuses on recent developments in peridynamics, nonlocal and fractional diffusion, and other related nonlocal models.

Organizer: Marta D'Elia
Sandia National Laboratories, USA

Organizer: Qiang Du
Columbia University, USA

Organizer: Pablo Seleson
Oak Ridge National Laboratory, USA

4:25-4:45 A Fractional Laplacian-Based Closure Model for Turbulent Fluid Flows

Max Gunzburger, Florida State University, USA; Nan Jiang, Missouri University of Science and Technology, USA; Feifei Xu, Florida State University, USA

4:50-5:10 Nonlocal Transport in Bounded Domains

Diego del-Castillo-Negrete, Oak Ridge National Laboratory, USA

continued on next page

5:15-5:35 Optimization with Respect to Order in a Fractional Diffusion Model: Analysis and Approximation

Abner J. Salgado, University of Tennessee, USA; Enrique Otarola, Universidad Técnica Federico Santa María, Chile; Harbir Antil, George Mason University, USA

5:40-6:00 An Efficient Probabilistic Numerical Method Based on Fourier-Cosine Series for Fractional Laplacian Equations

Guannan Zhang, Oak Ridge National Laboratory, USA

Thursday, March 2

MS251

Numerical Methods for Uncertainty Quantification, Surrogate Models, and Bayesian Inference - Part III of III

4:25 PM-6:05 PM

Room:203

For Part 2 see MS224

It is increasingly important to equip a numerical model or simulation with estimates of uncertainty. For these estimates to be meaningful, they must be carefully derived, e.g., by Bayes' rule and conditional probability, which allows one to estimate model uncertainties from noisy data. Numerical methods to perform such Bayesian inference often rely on Monte Carlo sampling. The cost if these methods can be high, because they require repeated evaluation of a numerical model, where each evaluation may be computationally expensive. This session focuses on techniques that aim to mitigate this computational burden, including replacing high-fidelity models with surrogate models, reducing the dimensionality of the parameter space, devising efficient sampling methods, and employing goal-oriented approaches.

Organizer: Matthias Morzfeld
Lawrence Berkeley National Laboratory, USA

Organizer: Fei Lu
Lawrence Berkeley National Laboratory, USA

Organizer: Kevin T. Carlberg
Sandia National Laboratories, USA

4:25-4:45 On a Formulation for Constructing Optimal Low-Rank Approximations with Respect to Goal Functionals

Serge Prudhomme and Kenan Kergrene, École Polytechnique de Montréal, Canada; Ludovic Chamoin, ENS Cachan, France; Olivier Le Maitre, LIMSI-CNRS, France; Marc Laforest, École Polytechnique de Montréal, Canada

continued in next column

4:50-5:10 Data Assimilation with Reduced Models

Fei Lu, Lawrence Berkeley National Laboratory, USA

5:15-5:35 Reduced-Order Modeling of Bayesian Inverse Problems for PDEs

Andrea Manzoni, École Polytechnique Fédérale de Lausanne, Switzerland; Stefano Pagani, Politecnico di Milano, Italy; Alfio Quarteroni, École Polytechnique Fédérale de Lausanne, Switzerland

5:40-6:00 Equation-Driven Probability Density Function Estimators for High-Dimensional Stochastic Dynamical Systems

Daniele Venturi, University of California, Santa Cruz, USA; Johannes O. Royset, Naval Postgraduate School, USA

Thursday, March 2

MS252

Advances in Adaptivity and Algorithms for Uncertainty Quantification

4:25 PM-6:05 PM

Room:204

Adaptive approaches and advanced algorithms provide a very effective and efficient way to perform reliable predictions for complex physical systems including stochastic systems that possess uncertainty or variability. This minisymposium will place emphasis on adaptive methods and advanced algorithms for uncertainty quantification (UQ). It will focus on topics that explore error estimation/indication, control of numerical error (and its impact on stochastic modeling), adaptive sampling, mesh adaptation and/or algorithms for next generation computing platforms.

Organizer: Onkar Sahni

Rensselaer Polytechnic Institute, USA

Organizer: Abani Patra

State University of New York at Buffalo, USA

4:25-4:45 Surrogate Construction and Adaptivity in Simulations/Sampling

Hossein Aghakahani and Abani Patra, State University of New York at Buffalo, USA; Elaine Spiller, Marquette University, USA

4:50-5:10 Variational Multiscale Method Based Error Estimation and Mesh Adaptivity for Intrusive UQ

Jason Li, Assad Oberai, and Onkar Sahni, Rensselaer Polytechnic Institute, USA

5:15-5:35 Basis and Sample Adaptive Polynomial Chaos Expansions

Jerrad Hampton and Alireza Doostan, University of Colorado Boulder, USA

5:40-6:00 Intrusive UQ Algorithms for Emerging Computing Platforms

Cosmin Safta, Habib N. Najm, and Eric Phipps, Sandia National Laboratories, USA

Thursday, March 2

MS253

Parallelizable Preconditioners and Iterative Solvers

4:25 PM-6:05 PM

Room:205

The continuous increase in computational power imposes a greater need for efficient scalable techniques for solving large sparse matrix systems. For iterative techniques, the efficiency of the solver largely depends on the implementation of a good parallelizable preconditioner. This minisymposium will present some of the recent work done on efficient solvers for PDE problems, as well as improvements toward solver composition. A number of preconditioning approaches will be presented, such as local incomplete factorization, multigrid and block preconditioners for systems arising from Helmholtz, (Navier) Stokes, Rayleigh-Benard, and optimization-based coupling problems.

Organizer: Artur Safin

University of Texas at Dallas, USA

Organizer: Susan Minkoff

University of Texas at Dallas, USA

4:25-4:45 Accurate Finite Element Solution of the Fully Coupled Thermoacoustic Equations for Modeling of Trace Gas Sensors

Artur Safin, Susan Minkoff, and John Zweck, University of Texas at Dallas, USA

4:50-5:10 Multigrid Preconditioning in Support of Optimization-Based Domain Decomposition for Elliptic Equations

Andrei Draganescu and Mona Hajghassem, University of Maryland, Baltimore County, USA

continued in next column

5:15-5:35 Preconditioners for Stokes Flow with Highly Heterogeneous Viscosity Structure: Saddle-Point Smoothing Via Local Incomplete Factorization

Patrick Sanan and Olaf Schenk, Università della Svizzera italiana, Switzerland; Matthias Bollhoefer, Technische Universität Berlin, Germany; Karl Rupp, Freelance Computational Scientist, Austria; Dave A. May, ETH Zürich, Switzerland

5:40-6:00 Solver Composition Across the PDE/Linear Algebra Barrier

Rob C. Kirby, Baylor University, USA; Lawrence Mitchell, Imperial College London, United Kingdom

Thursday, March 2

MS254

Efficient Iterative Solvers with Enlarged Minimization Spaces

4:25 PM-6:05 PM

Room:206

Krylov subspace solvers are very powerful tools to solve large linear systems, and in particular those arising from the discretization of partial differential equations. In some cases, convergence can be very slow or happen only after a long stagnation. These methods minimize a certain functional, such as a certain norm of the error at each iteration. A natural idea to accelerate them is to enlarge the minimization space. The aim of this minisymposium is to present some recently proposed methods based on this enlargement of the minimization space. These approaches include the use of deflated, multipreconditioned and block variants of the Krylov subspace methods.

Organizer: Nicole Spillane

Ecole Polytechnique, France

Organizer: Daniel B. Szyld

Temple University, USA

4:25-4:45 Enlarged GMRES

Hussam Al Daas, UPMC-Inria-TOTAL, France; Laura Grigori, Inria, France; Pascal Henon, Total E&P, France; Philippe Ricoux, TOTAL SA, France; *Olivier Tissot*, Inria, France

4:50-5:10 Adaptive Coarse Spaces for FETI-DP Domain Decomposition Methods

Axel Klawonn, and Kühn Martin, Universität zu Köln, Germany; Oliver Rheinbach, Technische Universität Bergakademie Freiberg, Germany

5:15-5:35 Adaptive Multipreconditioning and its Application to Domain Decomposition

Nicole Spillane, Ecole Polytechnique, France; Christophe Bovet, CNRS, Université Paris-Saclay, France; Pierre Gosselet, LMT-Cachan, France

5:40-6:00 Multipreconditioned GMRES for Shifted Systems

Tania Bakhos, Basque Center for Applied Mathematics, Spain; Peter K. Kitanidis, Stanford University, USA; Scott Ladenheim, Temple University, USA; Arvind Saibaba, Tufts University, USA; Daniel B. Szyld, Temple University, USA

continued in next column

Thursday, March 2

MS255

Recent Development of Verified Numerical Computations

4:25 PM-6:05 PM

Room:209

This minisymposium is devoted to verified numerical computations related to self-validating methods and computer-assisted proofs. Since verified numerical computations enable us to rigorously solve systems of equations by numerical methods in finite precision arithmetic such as floating-point arithmetic, they became increasingly important in a wide range of science and engineering. The main objective of the minisymposium is to discuss several recent topics on verified numerical computations and related numerical methods.

Organizer: Takeshi Ogita

Tokyo Woman's Christian University, Japan

Organizer: Siegfried M. Rump

Technische Universität, Hamburg-Harburg, Germany

4:25-4:45 Iterative Refinement for Eigenvectors of Symmetric Matrices with Clustered Eigenvalues

Takeshi Ogita, Tokyo Woman's Christian University, Japan; Kensuke Aishima, University of Tokyo, Japan

4:50-5:10 A Parallel Compensated Horner Scheme

Stef Graillat, University Pierre and Marie Curie (UPMC), France

5:15-5:35 Verified Solution of Unconstrained and Constrained Nonlinear Global Optimization Problems

Siegfried M. Rump, Technische Universität, Hamburg-Harburg, Germany

5:40-6:00 Verified Conic Solutions of Underdetermined Linear Systems

Marko Lange, Waseda University, Japan

Thursday, March 2

MS256

Advanced Computational Methods for Embedded Interfaces and Boundaries - Part II of II

4:25 PM-6:05 PM

Room:210

For Part 1 see MS229

Embedded/immersed boundary methods obviate the need for continual re-meshing in many applications involving rapid prototyping and design. A number of new methodologies have been recently developed, ranging from finite difference to finite element methods, in which remedies to some long standing problems regarding stability, robustness, accuracy, and flexibility have recently been introduced. This minisymposium attempts to bring together members of various scientific communities to present their most recent advances in this field. Applications include but are not confined to fluid and solid mechanics, fluid/structure interaction, multiphase flows, electromagnetics, radiation, etc.

Organizer: Guglielmo Scovazzi

Duke University, USA

Organizer: Alex Main

Duke University, USA

4:25-4:45 An Embedded Boundary Method for Shock-Dominated Fluid-Solid Interaction Problems

Kevin Wang, Yeyue Xiong, and Shunxiang Cao, Virginia Tech, USA; Pei Zhong and Ying Zhang, Duke University, USA

4:50-5:10 Coupled FEM-DEM Methods for Modeling Variably Saturated Granular Media

Chris Kees and Matthew Farthing, U.S. Army Engineer Research and Development Center, USA

5:15-5:35 Over-Coming Fluid-Structure Instabilities for Incompressible Flows and Light Bodies

William D. Henshaw, Rensselaer Polytechnic Institute, USA

5:40-6:00 An Immersed Structural Potential Method Framework for Incompressible Flexible/Rigid/Multi-Phase Flow Interaction

Antonio Gil and L. Yang, Swansea University, United Kingdom; Javier Bonet, University of Greenwich, United Kingdom

Thursday, March 2

MS257

Advances in Nonstandard Finite Element Methods for Interface Problems - Part II of II

4:25 PM-6:05 PM

Room:211

For Part 1 see MS230

Real-world applications involving multiple materials or physics often lead to the so-caller interface problems. Solution to interface problems involves kinks, discontinuities, singularities, and other non- smooth features. In past decades, many nonstandard finite element methods (FEM) have been developed to solve interface problems efficiently, such as Generalized/Extended FEM, Nitche's FEM, Immersed FEM. This minisymposium will bring together experts in these fields to discuss recent advances in developing and analyzing nonstandard finite element methods for interface problems.

Organizer: Xu Zhang

Mississippi State University, USA

Organizer: Uday Banerjee

Syracuse University, USA

4:25-4:45 Robust Flux Error Estimation of Nitsche's Methods for High Contrast Interface Problems

John Guzman, Brown University, USA; Erik Burman, University of Sussex, United Kingdom; Manuel Sanchez-Uribe, University of Minnesota, USA; Marcus Sarkis, Worcester Polytechnic Institute, USA, and Instituto de Matematica Pura e Aplicada (IMPA), Brazil

4:50-5:10 Improved ZZ a Posteriori Error Estimation of Conforming FEM for Diffusion Problems

Cuiyu He, Purdue University, USA

5:15-5:35 Composite Finite Elements

Stefan Sauter, University of Zurich, Switzerland

5:40-6:00 Error Estimates for Immersed Finite Element Volume Methods

Xu Zhang, Mississippi State University, USA; Qingsong Zou, Sun Yat-Sen University, China

Thursday, March 2

MS258

Innovative Time Integrators for Large-Scale Complex Problems - Part II of II

4:25 PM-6:05 PM

Room:212

For Part 1 see MS231

Many complex systems in science and engineering require numerical solution of evolution equations that describe their dynamics over time. Many of these systems involve a wide spectrum of spatial and temporal scales, which makes numerical solution of the corresponding equations a difficult task. Over the past several decades many novel time integration techniques have been introduced to address these challenges. The goal of this minisymposium is to present some of the latest developments in numerical time integration. The minisymposium will connect numerical analysts working in time integration with practitioners and researchers from other fields of computational science and engineering.

Organizer: Vu Thai Luan

University of California, Merced, USA

Organizer: Mayya Tokman

University of California, Merced, USA

4:25-4:45 Solving the Vlasov-Maxwell System in the Classical Limit

Lukas Einkemmer, University of Innsbruck, Austria

4:50-5:10 New Approach to Simulation of Elastodynamics Systems

Vu Thai Luan, University of California, Merced, USA; Dominik Michels, Stanford University, USA; Mayya Tokman, University of California, Merced, USA

5:15-5:35 EPIRK-K: A Fusion of EPIRK and K-Methods Theory

Mahesh Narayanamurthi, Paul Tranquilli, and Ross Glandon, Virginia Tech, USA; Mayya Tokman, University of California, Merced, USA; Adrian Sandu, Virginia Tech, USA

5:40-6:00 Parallel Exponential Integrators Based on General Linear Methods

Tommaso Buvoli, University of Washington, USA

Thursday, March 2

MS259

New Developments in Time-Stepping Strategies for Diffusive-Type Differential Equations

4:25 PM-6:05 PM

Room:213

Diffusive phenomena are ubiquitous in nature and in engineering applications. Two particular properties are 1) dependence on quantities far in the past ("history-dependence") and a 2) distinction between singular behavior at "short" times and smooth behavior at "long" times. These two properties make discretization of the underlying governing equations challenging. In this minisymposium, we will hear about new developments in discretization strategies for parabolic equations and fractional diffusion equations.

Organizer: Jing-Rebecca Li
INRIA Saclay, France

4:25-4:45 Fast Galerkin Bem for Parabolic Moving Boundary Problems
Johannes Tausch, Southern Methodist University, USA

4:50-5:10 A FEniCS-HPC Framework for Simulating Diffusion in Heterogeneous Media
Dang Van Nguyen, Johan Jansson, and Johan Hoffman, KTH Royal Institute of Technology, Sweden; Jing-Rebecca Li, INRIA Saclay, France

5:15-5:35 High-Order Adaptive Kernel Compression Time-Stepping Methods for Fractional Differential Equations
Daniel H. Baffet and Jan S. Hesthaven, École Polytechnique Fédérale de Lausanne, Switzerland

5:40-6:00 An Efficient Algorithm for Solving Fractional Diffusion Equations
Jiwei Zhang, Beijing Computational Science Research Center, China

Thursday, March 2

MS260

Meshless, Particle, and Particle-Mesh Methods for PDEs - Part I of II

4:25 PM-5:40 PM

Room:214

For Part 2 see MS286

Due to their inherent scalability, meshless, particle-based and particle-mesh methods are becoming increasingly important with recent increases in available computing power. Meshless and particle-based methods provide adaptive solutions for problems with deforming interfaces, without the burden of generating boundary conforming meshes. Particle and particle- mesh methods become critically important as scientific and engineering applications move towards more resolved / first principles approaches. In addition to classical applications of particle methods for PDEs in electromagnetism and cosmology, new applications in climate, energy, and environmental areas are adopting particle and hybrid methods. We focus on recent developments using these methods to scalably solve PDEs with diverse applications to scientific and engineering problems. In particular, a spectrum of methods will be represented: Lagrangian particle methods for hydrodynamic problems, recent advances in smoothed particle hydrodynamics, staggered moving least squares, PIC methods for plasma physics problems, as well as topics from scattered data approximation theory. Research issues of particular interest include rigorous foundations of methods based on mathematical approximation theory, error analysis and convergence, improved kernels and high order methods, spatial and temporal adaptivity, and scalability on modern supercomputer architectures.

Organizer: Alexandre M. Tartakovsky
Pacific Northwest National Laboratory, USA

continued in next column

Organizer: Roman Samulyak
Stony Brook University, USA

4:25-4:45 SPH Approximations of Stochastic Boundary Value Problems
Alexander Tartakovsky, Pacific Northwest National Laboratory, USA

4:50-5:10 Coupled Fluid-Solid-Fracture Using SPH
John R. Williams, Massachusetts Institute of Technology, USA

5:15-5:35 Massively Parallel Sph Simulations and Laboratory Experiments of Fracture Flow Dynamics: Toward the Process Understanding of Gravitational Driven Flows in Unsaturated Fractured Media
Jannes Kordilla, University of Goettingen, Germany

Thursday, March 2

MS261

How to Succeed with Open Source Scientific Software

4:25 PM-6:05 PM

Room:215

The open source model holds great promise for CSE software. Diverse contributions and peer reviews improve technical quality, distributed teams contribute developer horsepower, integration and testing in myriad environments improve software quality, and the open source code itself allows flexibility to tailor to new applications. Open source CSE software fosters open, reproducible research and supports an open science process. Yet achieving truly collaborative and open software can be challenging. Representing exemplar software projects, the speakers in this session will emphasize benefits and challenges of open source CSE software, and advise on best practices to succeed in collaborative development.

Organizer: Brian M. Adams

Sandia National Laboratories, USA

Organizer: Damon McDougall

University of Texas at Austin, USA

4:25-4:45 Code as a Research Product: Open Source for Open Science

J. Daniel Gezelter, University of Notre Dame, USA

4:50-5:10 Continuous Integration For Large-Scale Scientific Software Development

Cody J. Permann, Idaho National Laboratory, USA

5:15-5:35 Community Building and its Impact on Sustainable Scientific Software

Matthew J. Turk, University of Illinois at Urbana-Champaign, USA

5:40-6:00 15 Years of Trilinos: What Has Worked and Not

James Willenbring and Michael Heroux, Sandia National Laboratories, USA

Thursday, March 2

MS262

The Mori-Zwanzig Formulation and Its Application to Nonlinear Dynamical Systems

4:25 PM-6:05 PM

Room:216

The Mori-Zwanzig (MZ) formulation is a coarse-graining technique from irreversible statistical mechanics to formally integrate out an arbitrary number of phase variables in nonlinear dynamical systems. This methodology yields exact evolution equations for quantities of interest which would allow us to avoid integration of the full system (possibly high-dimensional), thus reducing the computational cost significantly. Computing the solution to the Mori-Zwanzig equation, however, is a challenging task that relies on approximations and appropriate numerical schemes. Over the years many different techniques have been proposed for this scope, with the most efficient ones being problem-specific. This minisymposium invites contributions that showcase the potential and effectiveness of the Mori-Zwanzig formulation in applied sciences, including particle models and multi-scale stochastic dynamical systems.

Organizer: Daniele Venturi

University of California, Santa Cruz, USA

4:25-4:45 Duality and Conditional Expectations in Nakajima-Mori-Zwanzig

Jason Dominy and Daniele Venturi, University of California, Santa Cruz, USA

4:50-5:10 Empirical Approaches to the Mori-Zwanzig Formalism

Fei Lu, Lawrence Berkeley National Laboratory, USA; *Kevin K. Lin*, University of Arizona, USA; Alexandre Chorin, University of California, Berkeley, USA

5:15-5:35 When Big Computers Are Not Enough: Model Reduction and Mesh Refinement

Panos Stinis, Pacific Northwest National Laboratory, USA

5:40-6:00 Data-Driven Stochastic Parameterization of Multiscale Dynamical Systems

John Harlim, Pennsylvania State University, USA

Thursday, March 2

MS263

Tripping on Data Collections: A Supercomputing Administrators Journey

4:25 PM-6:05 PM

Room:217

A computational facility presents challenges in archiving as they implement new technologies that gather data about power, temperature, humidity, I/O and presents unique opportunities for analysis and visualization. Where data points every five minutes were adequate to react to most situations, when we transition to a model of proactive monitoring and problem resolution, a stream of data points at 15,000 per second now becomes a big data challenge. This symposium features speakers who explored ways to analyze and visualize this data to improve processes in making decisions for an HPC data center operations whose challenges include collection, transportation, archiving, monitoring and querying of the data. Traditional methods can solve some of the challenges and others could not meet the full demand of the collection and analysis needs. Some of the novel approaches in analyzing this data include creating summary datasets which increased the amount of raw data gathered, intelligent tagging of the data to allow better sorting, processing and usages of the data and visualizing through direct data streaming to eliminate database queries. The group continues investigating new ways to visualized large and diverse datasets. The bigger challenge is to verify the data and determine the mathematical formulas to pare down the large amount of data in order to even begin analyzing it to leverage any efficiencies.

Organizer: Elizabeth Bautista

Lawrence Berkeley National Laboratory, USA

continued on next page

4:25-4:45 Herding Cats & Elks: Big-Plans with Big-Data and HPC Administration
Elizabeth Bautista, Lawrence Berkeley National Laboratory, USA

4:50-5:10 Old-School Hipsters Crash Big-Data's Party
Mark Sing, Lawrence Berkeley National Laboratory, USA

5:15-5:35 What the 'Heka' is Freeboard? Dynamic Visualizations
Jasmine Farrell, Lawrence Berkeley National Laboratory, USA

5:40-6:00 Laser-Swords into Data-Shares: Game Engines for Interactive Visualization
Eric Zimmerman, Lawrence Livermore National Laboratory, USA

Thursday, March 2

MS264

The Back-Box Approach to Exploring and Designing with Simulations

4:25 PM-6:05 PM

Room:218

Scientists, engineers, and decision makers increasingly rely on the results of computational simulations. Accordingly, it has become ever more important to ensure that simulation-based designs are optimal and feasible, that margins and uncertainty are accurately characterized, and that overall simulation credibility can be confidently stated. A wealth of resources exists for achieving these goals in the form of efficient algorithms for optimization, sensitivity analysis, and uncertainty quantification. However, engineering and science practitioners often lack the domain expertise needed to incorporate these algorithms into their computational codes, or the codes may be closed source, preventing an intrusive or close coupling. Contributors to this minisymposium will present applications-focused results in distinct engineering and science domains that illustrate the power and flexibility of a non-intrusive or "black-box" approach for simulation-based exploration and design. Each uses features of the Dakota toolbox, an open-source software project that provides a convenient interface to a range of well-established and cutting edge algorithms for optimization, sensitivity analysis, and uncertainty quantification.

Organizer: Adam Stephens

Sandia National Laboratories, USA

4:25-4:45 Dakota: Algorithms for Design Exploration and Simulation Credibility
Adam Stephens, Sandia National Laboratories, USA

continued in next column

4:50-5:10 Beyond Parameter Scans, Using Dakota for Real World Problems
Sharon Petney and John H. Carpenter, Sandia National Laboratories, USA; Robert L. Doney, III, U.S. Army Research Laboratory, USA

5:15-5:35 Uncertainty Quantification with Dakota and Nasa's Overflow2 CFD Solver within an in Situ Based Workflow
Brad Whitlock, Lawrence Livermore National Laboratory, USA; *Earl P. N. Duque,* Intelligent Light, USA

5:40-6:00 An Open-Source Framework for Multi-Physics Simulations and Design Optimization
Joel Guerrero, University of Genoa, Italy

Thursday, March 2

MS265

Sparse, Direct Solvers for Large-Scale Systems and Applications

4:25 PM-6:05 PM

Room:219

Modern applications require the solution of larger and larger sparse linear systems, with possibly in some cases, large numbers of right-hand sides. On the other side, supercomputers are increasingly complex due to their increasing number of compute nodes and to the use of multicore technologies and accelerators. Sparse, direct solvers are commonly appreciated for their robustness, reliability and ease of use. Nevertheless, they can be demanding both in execution time and memory consumption and the complexity of the associated workload makes their scalability challenging. In this workshop we present some recent advances that aim to reduce the cost of sparse, direct solvers as well as to improve their efficiency and scalability for large scale systems and applications.

Organizer: Theo Mary

Universite de Toulouse, France

Organizer: Wissam M. Sid-Lakhdar

Texas A &M University, USA

4:25-4:45 Comparison of BLR and HSS Low-Rank Formats in Multifrontal Solvers: Theory and Practice

Patrick Amestoy, ENSEEIHT-IRIT, France; Alfredo Buttari, CNRS, France; Pieter Ghysels, Lawrence Berkeley National Laboratory, USA; Jean-Yves L'Excellent, Inria-LIP-ENS Lyon, France; Xiaoye Sherry Li, Lawrence Berkeley National Laboratory, USA; *Theo Mary*, Universite de Toulouse, France; François-Henry Rouet, Lawrence Berkeley National Laboratory, USA

continued in next column

4:50-5:10 On the Solution Phase of Sparse Direct Solvers with Many Right-Hand Sides

Gilles Moreau, ENS Lyon, France; Jean-Yves L'Excellent, Inria-LIP-ENS Lyon, France; Patrick Amestoy, ENSEEIHT-IRIT, France

5:15-5:35 Scalable Sparse Direct Solver for Hybrid Architectures

Piyush Sao, Georgia Institute of Technology, USA; Xiaoye S. Li, Lawrence Berkeley National Laboratory, USA; Richard Vuduc, Georgia Institute of Technology, USA

5:40-6:00 Auto-Tuning for Multifrontal Sparse QR Factorizations on GPU

Wissam M. Sid-Lakhdar and Tim Davis, Texas A&M University, USA

Thursday, March 2

MS266

Advances in Reproducing Kernel Hilbert Spaces Applied to Bayesian Optimization

4:25 PM-6:05 PM

Room:220

Positive definite kernels (also referred to as reproducing kernels or radial basis functions) play an important role in fields as diverse as function approximation, numerical differential equations and machine learning. One role, which has received increased attention as data science becomes more powerful, is as covariance kernels in a Gaussian process regression. The machine learning strategies which power modern data analysis require tuning of their hyperparameters to reach optimal behavior; using a Gaussian process to model the impact of these hyperparameters has provided an efficient strategy to conduct this tuning. This black-box strategy is often referred to as Bayesian optimization, and this minisymposium contains talks on recent research in positive definite kernels and Bayesian optimization.

Organizer: Michael McCourt

SigOpt, USA

4:25-4:45 Failure Region Identification Coincident to Bayesian Optimization

Michael McCourt, SigOpt, USA; Ling Leevan, Hong Kong Baptist University, Hong Kong

4:50-5:10 Knowledge Gradient for Multi-Information Source Optimization

Peter I. Frazier and Jialei Wang, Cornell University, USA

5:15-5:35 Hierarchically Compositional Kernels for Regression and Parameter Estimation

Jie Chen, IBM T.J. Watson Research Center, USA

5:40-6:00 Iterated Brownian Bridge Kernels for Sequential Kriging Optimization

Greg Fasshauer, Colorado School of Mines, USA

Thursday, March 2

MS267

Molecular Solvation: New Methods and Applications

4:25 PM-6:05 PM

Room:Crystal AF - 1st Fl

Solvation remains an important phenomenon in many disciplines including chemistry, biology, and biomedical engineering. The computational challenges associated with particle-based treatments of solvents has necessitated the development of other methods and models. Traditional continuum theories based on macroscopic ideas, such as dielectric response, have been largely limited to predicting simple quantities such as energies. In this minisymposium we present recent approaches and applications of solvation phenomena, including both classical and multiscale approaches, as well as methods that allow predictions of additional thermodynamic and transport properties that were previously unavailable.

Organizer: Ahmed E. Ismail

West Virginia University, USA

4:25-4:45 Recent Advances in Atomistic Simulations of Biomass Dissolution

Ahmed E. Ismail, West Virginia University, USA; Brooks Rabideau, University of South Alabama, USA; Pan Chen, KTH Royal Institute of Technology, Sweden; Yoshiharu Nishiyama, Université de Grenoble Alpes, France

4:50-5:10 Towards a Molecular Level Understanding Hydration Lubrication: Structure and Dynamics of 2-Methacryloyloxyethyl Phosphorylcholine

Christoph Klein, William Roussell, Christopher Iacovella, and Clare McCabe, Vanderbilt University, USA; Peter Cummings, Oak Ridge National Laboratory, USA

continued in next column

5:15-5:35 Evaporation-Induced Nanoparticle Assembly

Shengfeng Cheng, Virginia Tech, USA

5:40-6:00 Including First-Shell Response in Continuum Solvent Models Using Multiscale Boundary Conditions

Jaydeep P. Bardhan, Amirhossein Molavi Tabrizi, Ali Mehdizadeh Rahimi, and Spencer Goossens, Northeastern University, USA; Matthew G. Knepley, Rice University, USA

Thursday, March 2

MS268

Data Methods for Complex Systems

4:25 PM-6:05 PM

Room:Crystal CD - 1st Fl

Across the engineering and natural sciences, data is increasingly abundant, due to revolutionary advances in sensor technology, data storage and transfer, and computational capabilities. At the same time, many modern problems of interest are not readily analyzed from first principles, so that data-driven approaches are becoming the first line of attack. In this session, invited experts will discuss the application of methods from machine learning and compressed sensing to dynamical systems and control. These ideas will be developed in the context of societally important applications including turbulence control, modeling and suppressing the spread of disease, and machine vision.

Organizer: Steven Brunton

University of Washington, USA

Organizer: Nathan Kutz

University of Washington, USA

4:25-4:45 Nonlinear System Identification for Complex Systems

Joshua L. Proctor, Institute for Disease Modeling, USA

4:50-5:10 Randomized Matrix Decompositions for High-Dimensional Dynamic Data

Benjamin Erichson, University of St. Andrews, United Kingdom; Sergey Voronin, Tufts University, USA

5:15-5:35 Data-Based Extraction of Modal Interaction Networks

Aditya G. Nair and Kunihiko Taira, Florida State University, USA; Steven Brunton, University of Washington, USA

5:40-6:00 Model Inference in Epidemiology and Biological Networks Using Sparse Identification of Nonlinear Dynamics

Niall M. Mangan, University of Washington, Seattle, USA

Thursday, March 2

MS269

Advancing Cross-Cutting Ideas for Computational Climate Science

4:25 PM-6:05 PM

Room:301

As the climate science community explores a host of critical science questions to be answered over the next 10+ years, with the aim of informing stakeholders about the ongoing changes in global and local climate, there is a growing recognition of the expanding requirements for multiscale, global, coupled Earth system models. They are expected to provide much more detail and fidelity, with a much better understanding of their uncertainties, while still executing robustly and efficiently on ever larger and more complex computing systems. This requires fresh thinking that will mold the optimal science directions and motivate the latest and as yet to be uncovered developments in applied mathematics and computer science that will be required to handle new requirements. There is a recent effort that brings together computational climate scientists, applied mathematicians and computer scientists to generate such fresh thinking. This minisymposium will give an overview of the outcome of the effort.

Organizer: Esmond G. Ng

Lawrence Berkeley National Laboratory, USA

Organizer: Katherine J. Evans

Oak Ridge National Laboratory, USA

4:25-4:45 A Case for Cross-Cutting Ideas for Computational Climate Science

Katherine J. Evans, Oak Ridge National Laboratory, USA; Esmond G. Ng, Lawrence Berkeley National Laboratory, USA

continued in next column

4:50-5:10 A Multiscale Integrated Modeling Framework for Climate Science

Ruby Leung, Pacific Northwest National Laboratory, USA

5:15-5:35 Applied Mathematics and Computational Opportunities for Climate Science

Stefan Wild, Argonne National Laboratory, USA; George Ostrouchov, Oak Ridge National Laboratory, USA; Daniel Martin, Lawrence Berkeley National Laboratory, USA; Ray S. Tuminaro, Sandia National Laboratories, USA; Sam Williams, Lawrence Berkeley National Laboratory, USA; Kerstin Kleese Van Dam, Brookhaven National Laboratory, USA

5:40-6:00 Quantifying Uncertainties in Climate Science

Charles Jackson, University of Texas at Austin, USA

Thursday, March 2

MS270

Data Analysis and Workflows for Structural Descriptions of Complex Materials

4:25 PM-6:05 PM

Room:302

New types of highly complex materials - amorphous, highly-disordered, and hierarchically structured materials - constitute a serious challenge to the nation's ambitious Materials Genome Initiative (MGI). MGI aims to cut in half the time for new materials to move from the laboratory to the market by using an unprecedented synthesis of experimental and computational techniques. While this combination of experiment and high-performance computing will be essential for future breakthroughs in materials, it is also clear that such discoveries will depend upon our ability to process, analyze, and thoroughly explore large simulation and experimental data sets. Unfortunately, in many cases involving highly complex materials, the data are already too big to handle using current software and analytical processes. Unlike the case for well-ordered crystalline materials, in the case of highly disordered materials, the data analysis toolkit is all but completely empty. The research presented in this minisymposium fills this critical gap in MGI research infrastructure for disordered materials through application-driven software research on data generated in a technologically promising class of materials, known as High Entropy Alloys (HEAs). HEAs, composed of a minimum of five principal elements, pose a particularly robust test of the proposed algorithms because the corresponding materials discovery process requires a relatively high-dimensional optimization through composition space.

Organizer: Piotr Luszczek

University of Tennessee, USA

continued on next page

4:25-4:45 Deviation from High-Entropy Configurations in the $Al_{1.3}$ CoCrCuFeNi Alloy
Peter Liaw, University of Tennessee, USA

4:50-5:10 Advanced Particle Filters for Stochastic Point Set Registration
Vasileios Maroulas, University of Tennessee, Knoxville, USA

5:15-5:35 Algorithms for 3D-3D Registration with Known and Unknown References: Applications to Materials Science
David J. Keffer and Nicholas McNutt, University of Tennessee, USA

5:40-6:00 Implementation Techniques for Point Set Registration on Multicore and Hetergoneneous Hardware
Piotr Luszczek, University of Tennessee, USA

Thursday, March 2

MS271

Advances in Quantification of Uncertainty in Chemical and Material Systems

4:25 PM-6:05 PM

Room:303

One of the outstanding challenges in multi-scale modeling in applications such as chemical networks or materials is dealing with uncertainty for high-dimensional model parameters, and the physical models themselves which are fundamentally nonlinear, stochastic and multi-scale. Without proper mathematical and computational formulations and framework for model reduction or scalable reduced-order stochastic representation, the prohibitive computational cost for inclusion of UQ in multi-scale modeling cannot be addressed. In this minisymposium, novel mathematical approaches for sensitivity analysis based on information measures, sparse multi-scale algorithms for material failure and data-driven approaches for computing probability of failure will be presented.

Organizer: Miroslav Stoyanov

Oak Ridge National Laboratory, USA

4:25-4:45 Quantifying Probability of Failure Based on Noisy Multi-Fidelity Data
Maziar Raissi, Brown University, USA; Paris Perdikaris, Massachusetts Institute of Technology, USA; George Em Karniadakis, Brown University, USA

4:50-5:10 Uncertainty Quantification for Electronic-Structure-Based Chemical Kinetics Modeling
Markos A. Katsoulakis, University of Massachusetts, Amherst, USA

5:15-5:35 Predicting Fracture Patterns in Simulations of Brittle Materials under Variable Load and Material
Miroslav Stoyanov, Oak Ridge National Laboratory, USA

5:40-6:00 Accelerated Sampling and Sensitivity Estimation of Multiscale Reaction Networks
Ting Wang and Petr Plechac, University of Delaware, USA

Thursday, March 2

MS272

Recent Advances in Computational Subsurface Hydraulic Modeling and Analysis

4:25 PM-6:05 PM

Room:221

Modeling and analysis of groundwater flow in geologic media covers a wide range of computational issues related to model calibration and reduction, data assimilation, uncertainty quantification, and decision support to name a few. In this session, we want to bring together researchers from various aspects of groundwater modeling and analysis to discuss the recent advances and challenges arising from different applications. The purpose is to demonstrate the importance of computational techniques in understanding and analyzing the groundwater models. Computational issues such as regularization theory, numerical optimization and machine learning techniques will be discussed.

Organizer: Youzuo Lin

Los Alamos National Laboratory, USA

Organizer: Velimir V. Vesselinov

Los Alamos National Laboratory, USA

4:25-4:45 Hybrid First-Principles Data-Driven Dynamic Model Misspecification Correction
Lior Horesh and Theodore Van Kessel, IBM Research, USA; Omolade Saliu, IBM, Canada; Andrew R. Conn, IBM T.J. Watson Research Center, USA

4:50-5:10 Characterization of Poromechanical Behavior of Faulted Reservoirs During Injection-Induced Seismicity Using a Bayesian Inversion Approach
Birendra Jha, University of Southern California, USA; Jayanth Jagalur-Mohan, Zheng Wang, Ruben Juanes, and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

continued on next page

Thursday, March 2

MS272

Recent Advances in Computational Subsurface Hydraulic Modeling and Analysis

4:25 PM-6:05 PM

continued

5:15-5:35 Bayesian Inversion for Subsurface Properties from Poroelastic Forward Models and Surface Deformation Data

Amal M. Alghamdi, Marc A. Hesse, and Omar Ghattas, University of Texas at Austin, USA

5:40-6:00 Hydraulic Inverse Modeling Using Total-Variation Regularization with Relaxed Variable-Splitting

Youzuo Lin, Velimir V. Vesselinov, Dan O'Malley, and Brendt Wohlberg, Los Alamos National Laboratory, USA

Thursday, March 2

MS273

Quantifying Errors and Uncertainty in Inadequate Models for Complex Physics

4:25 PM-6:05 PM

Room:222

It is commonplace that models for physical systems are inadequate i.e. output from the model is significantly different from experimentally or naturally-observed quantities. When making predictions in regimes where observations are unavailable, it is important to remain cognizant of uncertainty not only in the model parameters and the observations used for calibration, but also in the sub-model for the inadequacy. This minisymposium will focus on the coupled aspects of uncertainty quantification and modeling error for physical systems in a Bayesian context.

Organizer: Manav Vohra
University of Texas at Austin, USA

4:25-4:45 Quantifying Uncertainty in Predictions from Inadequate Models for Porous Media Transport

Manav Vohra, Damon McDougall, Todd A. Oliver, and Robert D. Moser, University of Texas at Austin, USA

4:50-5:10 A Hierarchical Bayesian Approach for Characterizing Model Bias

Chi Feng, Massachusetts Institute of Technology, USA

5:15-5:35 Stochastic Simulation of Predictive Space-Time Scenarios of Wind Speed Using Observations and Physical Models

Julie Bessac, Emil M. Constantinescu, and *Mihai Anitescu*, Argonne National Laboratory, USA

5:40-6:00 Approximate Bayesian Inference for Intractable Likelihood Functions

Gabriel Terejanu, University of South Carolina, USA

Thursday, March 2

CP19

Life Sciences - Part II of II

4:25 PM-6:05 PM

Room:223

For Part 1 see CP17

Chair: To Be Determined

4:25-4:35 Dynamics of a Two-Vector, Two-Pathogen, Two-Host Model

Caleb L. Adams, Radford University, USA

4:37-4:47 Development of a Dynamical System for the Simulation of Immune Cells and Antigens

Rumana Ahmed, City College of CUNY, USA; Mahbubur Rahman, University of North Florida, USA

4:49-4:59 Robust Regulation of Hepatic Pericentral Amination by Glutamate Dehydrogenase Kinetics

Soumen Bera, P.hD Research Scholar, India

5:01-5:11 Scanning Electron Microscope Simulation with Adaptive Finite Elements

William F. Mitchell and John Villarrubia, National Institute of Standards and Technology, USA

Thursday, March 2

CP20

Computational Science Tools

4:25 PM-6:05 PM

Room:224

Chair: To Be Determined

4:25-4:35 An Interoperable Workflow Platform for Multi-Disciplinary Simulations

Kwai L. Wong, University of Tennessee and Oak Ridge National Laboratory, USA; Tanner Curren, Maryville College, USA

4:37-4:47 Systematic Modeling of Structured-Grid Numerical Applications for Automatic Parallelization

Aiqing Zhang, Institute of Applied Physics and Computational Mathematics, China; Zeyao Mo, CAEP Software Center for High Performance Numerical Simulations, China; Xiaolin Cao, Qinkai Liu, and Xiaowen Xu, Institute of Applied Physics and Computational Mathematics, China

4:49-4:59 Mathematical Modelling and Analysis for Making Career Decisions in Football Using Data Mining and Statistical Techniques

Parardha Kumar and Aakar Dwivedi, Indian School of Mines, India

5:01-5:11 An Experimental Investigation into the Practical Performance of Lattice Reduction Algorithms on Ideal Lattices

Scott C. Batson, Jamie R. Lyle, and Bryan Williams, SPAWAR Systems Center, USA; Kayla Capitan, Palmetto Scholars Academy, USA; Georgianna Campbell, University of Georgia, USA; Tuwaner Lamar, Morehouse College, USA; Hemant Pendharkar, Worcester State University, USA

5:13-5:23 Mapping of Language to a Logic Model Checker (LMC)

Colin James III, Ersatz Systems Machine Cognition, LLC, USA

continued in next column

5:25-5:35 Optimizing Structured-Grid Halo-Exchange Communications for Accelerator-Resident Computing on Multicore Platforms with Multiple MICs

Zhang Yang, Yang Yang, and Aiqing Zhang, Institute of Applied Physics and Computational Mathematics, China

5:37-5:47 Domain Management for Future Scale Parallelism

Christoph M. Ertl, Technische Universität München, Germany; Jérôme Frisch, RWTH Aachen University, Germany; Ralf-Peter Mundani and Ernst Rank, Technische Universität München, Germany

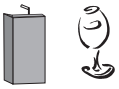
5:49-5:59 Performance Portability and Analysis of a Finite Element Multi-Physics Code

Jerry Watkins, Stanford University, USA; Irina Tezaur, Sandia National Laboratories, USA

Intermission

6:05 PM-6:20 PM

Business Meeting



6:20 PM-7:20 PM

Room:Ballroom C - 2nd Fl

Complimentary beer and wine will be served.

Open to SIAG/CSE members.

Friday, March 3

Registration

7:45 AM-12:00 PM

Room:Foyer - 1st Fl

Closing Remarks

8:00 AM-8:15 AM

Room:Grand Ballroom - 2nd Fl

IP9

Stochastic Gradient Methods for Machine Learning

8:15 AM-9:00 AM

Room:Grand Ballroom - 2nd Fl

Chair: Edmond Chow, Georgia Institute of Technology, USA

The stochastic gradient method has emerged as the most powerful technique for training the large-scale statistical models that form the foundation of modern machine learning systems. This talk provides an accessible introduction to the mathematical properties of stochastic gradient methods, and the intuition behind them. To set the stage, we present two case studies, one involving sparse linear models for text classification and one involving deep neural networks for image recognition. We then discuss advanced algorithms that control noise and make use of second order information. We conclude the talk with a discussion of the geometry of deep neural networks.

Jorge Nocedal
Northwestern University, USA

Intermission

9:00 AM-9:10 AM

Friday, March 3

MS199

Optimization Methods and Parallel Computing for Tensor Problems - Part I of II

9:10 AM-10:50 AM

Room:222

For Part 2 see MS225

Tensor (or higher-order matrix) naturally arises in applications that collect data along multiple dimensions (also called mode or way) such as in neuroimaging, multivariate statistics, multilinear algebra, data mining, speech recognition, to name a few. Since multi-way data can easily require terabytes, this makes it a great challenge for computation, data storage and transfer. Towards finding solutions of tensor problems efficiently, exploration of structures of the data, designing specific optimization methods, and also utilizing modern high-performance parallel computers are much needed. The two sessions will have recent developments along these lines.

Organizer: Yangyang Xu

University of Alabama, USA

Organizer: Carmeliza Navasca

University of Alabama at Birmingham, USA

9:10-9:30 Fast Algorithms for Higher-Order Singular Value Decomposition with Missing Data

Yangyang Xu, University of Alabama, USA

9:35-9:55 Shape Constrained Tensor Factorizations

Eric Chi, North Carolina State University, USA; Bethany Lunch and Nathan Kutz, University of Washington, USA

10:00-10:20 Distributed Nonnegative Tensor Low Rank Approximation for Large-Scale Clustering

Ramakrishnan Kannan, Oak Ridge National Laboratory, USA; Grey Ballard, Wake Forest University, USA; Barry Drake and Haesun Park, Georgia Institute of Technology, USA

10:25-10:45 The Tensor Approximation Problem from a Dynamical Systems Perspective

Martin J. Mohlenkamp, Ohio University, USA

Friday, March 3

MS274

Highly Scalable Solvers for Computational PDEs - Part I of II

9:10 AM-10:50 AM

Room:Grand Ballroom - 2nd Fl

For Part 2 see MS301

Efficient computational solution of high fidelity large-scale problems in computational science and engineering is still a major challenge. Complex applications include difficulties such as transient problems with widely varying time and spatial scales, strongly coupled multiphysics, heterogenous media, nonlinearlities, etc. The development of efficient linear system solvers for these classes of problems has many challenges, especially for high fidelity large-scale simulations, which makes proper preconditioning critical. This minisymposium will focus on highly scalable preconditioners, for example multigrid or domain decomposition approaches, multiphysics solvers (e.g. based on block factorization techniques), nonlinear preconditioning, multiscale solvers for heterogenous problems or space-time solvers, etc.

Organizer: Santiago Badia

Universitat Politecnica de Catalunya, Spain

Organizer: Paul Lin

Sandia National Laboratories, USA

9:10-9:30 Scalable Domain Decomposition Solvers for Embedded Boundary Methods

Santiago Badia, Universitat Politecnica de Catalunya, Spain; Francesc Verdugo, CIMNE, Spain

9:35-9:55 A User-Friendly Highly Scalable Amg Solver

Yvan Notay, Université Libre de Bruxelles, Belgium

10:00-10:20 An Algebraic Multigrid Approach to PDE Systems with Variable Degrees-of-Freedom Per Node

Raymond S. Tuminaro, Sandia National Laboratories, USA

10:25-10:45 Scaling Finite Element Multigrid Solvers to Ten Trillion (10^{13}) Unknowns

Dominik Bartuschat and *Ulrich J. Ruede*, University of Erlangen-Nuremberg, Germany

Friday, March 3

MS275

Reduced Models and Multiscale Methods - Part I of II

9:10 AM-10:50 AM

Room:Ballroom D - 2nd Fl

For Part 2 see MS302

Accurate and efficient simulations of physical responses in large-scale heterogeneous media is crucial to search and image geological formations in a wide range of geophysical applications, including mineral and hydrocarbon exploration, water resource utilizations, and geothermal power extractions. One major challenge in practice to perform this type of simulations is the excessive computational cost it involves. In this session we explore ways to reduce the complexity and the cost of the simulation by introducing multiscale and upscaling methods as well as reduce space modeling.

Organizer: Luz Angelica Caudillo Mata

University of British Columbia, Canada

Organizer: Eldad Haber

University of British Columbia, Canada

9:10-9:30 Multiscale and Upscaling Finite Volume Methods in Electromagnetic Geophysics

Luz Angelica Caudillo Mata, Eldad Haber, and Christoph Schwarzbach, University of British Columbia, Canada

9:35-9:55 Spectral Upscaling for Graph Laplacian Problems with Application to Reservoir Simulation

Andrew Barker, Lawrence Livermore National Laboratory, USA; *Chak Lee*, Texas A&M University, USA; Panayot Vassilevski, Lawrence Livermore National Laboratory, USA

10:00-10:20 Hybrid MultiScale Finite Element-Finite Volume Method for Poroelastic Geological Media

Nicola Castelletto, Stanford University, USA; Hadi Hajibeygi, Technical University of Delft, Netherlands; Hamdi Tchelepi, Stanford University, USA

Friday, March 3

MS276

Poroelasticity: Recent Theoretical and Computational Advances - Part I of II

9:10 AM-10:50 AM

Room:202

For Part 2 see MS303

Poroelasticity is the science of fluid-saturated, elastic, porous media (elastic solids) and the interactions between the fluid and the elastic porous structures. The equations of poroelasticity arise in diverse areas of science and technology, from geomechanics and geophysics to man made materials and biological tissue. Speakers will describe recent advances in the theoretical analysis and numerical approximation of solutions of the equations of poroelasticity and the analysis and simulation of related physical phenomena and the equations describing them.

Organizer: Yanzhao Cao

Auburn University, USA

Organizer: Amnon J. Meir

Southern Methodist University, USA

9:10-9:30 Direct and Inverse Problems for Biot's Equations

Viatcheslav I. Priimenko, North Fluminense State University, Brazil; Mikhail P. Vishnevskii, North Fluminense State University Darcy Ribeiro, Brazil and Sobolev Institute of Mathematics, Russia

9:35-9:55 Analysis of Nonlinear Poro-Visco-Elasticity with Applications to the Human Eye

Lorena Bociu, North Carolina State University, USA; Giovanna Guidoboni, Indiana University - Purdue University Indianapolis, USA; Riccardo Sacco, Politecnico di Milano, Italy; *Justin Webster*, College of Charleston, USA

10:00-10:20 Analysis of Partitioned Methods for the Biot System

William Layton, University of Pittsburgh, USA

10:25-10:45 Viscodynamic Operators in Poroelastic Wave Equations

Yvonne Ou, University of Delaware, USA

Friday, March 3

MS277

Numerical Methods for Wave Propagation and Its Applications - Part I of II

9:10 AM-10:50 AM

Room:203

For Part 2 see MS304

Fast and robust numerical methods for wave propagation play a key role in lots of problems with important applications, ranging from nano-optics to medical imaging. This minisymposium will discuss recent advances in the development of fast numerical algorithms for wave equations, as well as its applications in inverse problems and optimal design, creating the opportunity for collaboration between computational mathematics and other fields, such as optics, materials sciences, and imaging sciences.

Organizer: Min Hyung Cho

University of Massachusetts, Lowell, USA

Organizer: Jun Lai

Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Carlos Borges

University of Texas at Austin, USA

9:10-9:30 Numerical Solution to a Linearized Time Fractional KdV Equation on Unbounded Domains

Qian Zhang and Jiwei Zhang, Beijing Computational Science Research Center, China; *Shidong Jiang*, New Jersey Institute of Technology, USA; Zhimin Zhang, Beijing Computational Science Research Center, China

9:35-9:55 Optimal Design of Metallic Surfaces for Near-Field Energy Extraction

Owen D. Miller and *Yuxiang (Larry) Liu*, Yale University, USA

10:00-10:20 Inverse Medium Problem for Acoustic Problems

Carlos Borges, University of Texas at Austin, USA; Leslie Greengard, Courant Institute of Mathematical Sciences, New York University, USA; Adrianna Gillman, Rice University, USA

10:25-10:45 Scattering of Transient Waves by Piecewise Homogeneous Obstacles

Francisco J. Sayas, University of Delaware, USA; Alexander Rieder, Technische Universitaet Wien, Germany

Friday, March 3

MS278

Programming Scientific Codes on Recent Multicore and Manycore Processors - Part I of II

9:10 AM-10:50 AM

Room:204

For Part 2 see MS305

Efficient computation using multiple cores continues to be a challenge, especially as new manycore architectures enter the field, such as Intel Xeon Phi Knights Landing and the ShenWei processors used in TaihuLight. The speakers will demonstrate how to achieve high performance on different applications and platforms, including scheduling and balancing multiple threads on irregular workloads, paying attention to cache and memory in the context of large numbers of concurrent threads, and exploiting features of the processors such as special memory and vectorization.

Organizer: Edmond Chow

Georgia Institute of Technology, USA

Organizer: Xiaoye Sherry Li

Lawrence Berkeley National Laboratory, USA

9:10-9:30 MATLAB and MEX for Multicore Machines

Pat Quillen, MathWorks, USA

9:35-9:55 A Study on the Impact of Extra Precision on the Unsymmetric Eigenvalue Problem

Greg Henry, Intel Corporation, USA

10:00-10:20 Vectorizing and Multithreading the Calculation of Electronic Integrals

Benjamin Pritchard and Edmond Chow, Georgia Institute of Technology, USA

10:25-10:45 Preliminary Studies of an Implicit Navier-Stokes Solver on a Many-Core Machine

Rongliang Chen, Li Luo, and Ziju Liao, Chinese Academy of Sciences, China; Zhengzheng Yan, Shenzhen Institute of Advanced Technology, China; Xiao-Chuan Cai, University of Colorado Boulder, USA

Friday, March 3

MS279

Recent Advances in Unstructured Mesh Algorithms and Their Applications - Part I of II

9:10 AM-10:50 AM

Room:205

For Part 2 see MS306

Unstructured meshes continue to be ubiquitous in computational science and engineering simulations. In recent years, there have been some exciting developments in regards to unstructured mesh algorithms. For example, progress has been made in the areas of parallel mesh generation, high-order mesh generation, anisotropic adaptive meshing, and dynamic meshing to name just a few. Similarly, meshes have been employed in challenging simulations involving applications of fluid and solid mechanics, patient-specific medicine, design of materials, and computer graphics, and many others. The minisymposium will feature presentations on such algorithms and applications, as well as other related problems.

Organizer: Maurin A. Lopez Varilla

University of Kansas, USA

Organizer: Suzanne M. Shontz

University of Kansas, USA

9:10-9:30 A Global Optimization and Adaptivity-Based Algorithm for Automated Edge Grid Generation

Suzanne M. Shontz, University of Kansas, USA; David McLaurin, CD-adapco, USA

9:35-9:55 Portably Performant and Conservative Mesh Adaptivity for Lagrangian Shock Dynamics

Dan A. Ibanez and Mark S. Shephard, Rensselaer Polytechnic Institute, USA; Thomas Voth, Edward Love, James Overfelt, and Glen Hansen, Sandia National Laboratories, USA

continued in next column

10:00-10:20 Topology Optimization and Mesh Adaptation

Nicola Ferro, Simona Perotto, and Stefano Micheletti, Politecnico di Milano, Italy

10:25-10:45 A Flexible Conservative Remapping Framework for Exascale Computing

Ondrej Certik, Charles R. Ferenbaugh, R*ao V. Garimella*, Angela Herring, Brian Jean, Christopher Malone, and Christopher Sewell, Los Alamos National Laboratory, USA

Friday, March 3

MS280

Numerical Methods for Electronic Structure Calculations: Ground State Properties - Part I of II

9:10 AM-10:50 AM

Room:206

For Part 2 see MS307

The goal of this minisymposium is to bring experts working on numerical methods for electronic structure computations for materials together. In a wide range of applications, materials have to be studied at the quantum level. Among them, let us mention for instance conducting, magnetic or optical properties. The computation and characterization of the electronic structure of such materials raise numerous challenges from the mathematical and computational point of view, in particular due to the increasing complexity of the systems that are of interest to materials scientists. This minisymposium will focus more specifically on numerical methods for ground state calculations. The first talk of the session will give an introduction to ground state electronic structure computations and the other invited speakers will present their latest developments in the field.

Organizer: Virginie Ehrlacher

CERMICS, France

9:10-9:30 Advances in Real Space Methods to Solve the Kohn-Sham Equation

James R. Chelikowsky and Charles Lena, University of Texas at Austin, USA; Ariel Biller and Leeor Kronik, Weizmann Institute of Science, Israel

9:35-9:55 Title Not Available At Time Of Publication

Xiaoying Dai, Chinese Academy of Sciences, China

10:00-10:20 Electronic Transport in Incommensurate Van Der Waals 2D Heterostructures

Paul Cazeaux, University of Minnesota, USA

10:25-10:45 Band Structure Inverse Problem

Athmane Bakhta, École des Ponts ParisTech, France

Friday, March 3

MS281

Sensitivity Analysis and Uncertainty Quantification of Chaotic Systems - Part I of II

9:10 AM-10:50 AM

Room:209

For Part 2 see MS308

Chaotic dynamics appears in many scientific and engineering applications. Sensitivity analysis in the presence of chaos is challenging, but necessary to understand and control solution responses to variations in geometry, simulation parameters, and numerical discretization. Uncertainty quantification is needed to assess the accuracy and reliability of quantities predicted by chaotic dynamics simulations.

Organizer: Boris Diskin

National Institute of Aerospace, USA

Organizer: Eric Nielsen

NASA Langley Research Center, USA

9:10-9:30 Mathematical and Numerical Challenges in Shadowing Methods for Sensitivity Analysis of Chaotic Simulations

Qiqi Wang, Massachusetts Institute of Technology, USA

9:35-9:55 Simultaneous Parallel-in-Time Optimization with Unsteady PDEs Using a Multigrid Reduction in Time Software Library

Stefanie Günther and Nicolas R. Gauger, Technische Universität Kaiserslautern, Germany; Jacob B. Schroder, Lawrence Livermore National Laboratory, USA

10:00-10:20 Towards a Posteriori Error Estimation for Least Squares Shadowing Sensitivity Analysis of Chaotic Systems

Angxiu Ni and Qiqi Wang, Massachusetts Institute of Technology, USA

10:25-10:45 Uncertainty Estimates for Statistics Computed from Simulations of Chaotic Systems

Todd A. Oliver, Sigfried Haering, Nicholas Malaya, and Robert D. Moser, University of Texas at Austin, USA

Friday, March 3

MS282

Advances in Fast Solution of Sparse and Structured Linear Systems - Part I of II

9:10 AM-10:50 AM

Room:210

For Part 2 see MS309

This minisymposium concerns the numerical solution of sparse and structured linear systems. We provide an overview of recent advances in the field, spanning preconditioned iterative methods in parallel and sequential settings, matrix equations, innovative preconditioning approaches for partial differential equations, error bounds, and Krylov subspace iterative methods for saddle point systems.

Organizer: Jessica Bosch

University of British Columbia, Canada

Organizer: Chen Greif

University of British Columbia, Canada

9:10-9:30 A Minimum Residual Method for Saddle Point Systems

Chen Greif, University of British Columbia, Canada; Ron Estrin, Stanford University, USA

9:35-9:55 Estimating of the 2-Norm Forward Error for SYMMLQ and CG

Ron Estrin, Stanford University, USA; Dominique Orban, École Polytechnique de Montréal, Canada; Michael A. Saunders, Stanford University, USA

10:00-10:20 Parallel Versions of the Southwell Iterative Method with Low Communication for Preconditioning and Smoothing

Edmond Chow and Jordi Wolfson-Pou, Georgia Institute of Technology, USA

10:25-10:45 Matrix-Equation-Based Strategies for Certain Structured Algebraic Linear Systems

Valeria Simoncini, Universita' di Bologna, Italy

Friday, March 3

MS283

Coupling Strategies for PDEs - Part I of II

9:10 AM-10:50 AM

Room:211

For Part 2 see MS310

Interfaces may occur naturally when modeling physical systems in contact, or may occur artificially when used to capture material defects and small scale features in certain portions of the domain. Artificial interfaces can additionally occur when decomposing a domain to reduce computational load on each processor or when dealing with meshes for subdomains that have been generated independently. There exist a wide variety of codes for performing computational simulations of physical systems governed by partial differential equations, each having their own unique capabilities and strengths. Coupling algorithms for interfaces permit the most appropriate tool to be used dependent upon mesh and constitutive equation for each subdomain. This minisymposium aims to present research related to interface coupling methods including theoretical formulations and results from applications.

Organizer: Paul Kuberry

Sandia National Laboratories, USA

Organizer: Kara Peterson

Sandia National Laboratories, USA

9:10-9:30 Coupling Hyperbolic PDEs Over Non-Coincident Interfaces

Paul Kuberry, Kara Peterson, and Pavel Bochev, Sandia National Laboratories, USA

9:35-9:55 Non-Iterative Multi-Physics Domain Decomposition Method for Coupled Free Flow and Porous Media Flow Problem

Xiaoming He, Missouri University of Science and Technology, USA

10:00-10:20 An Explicit Partitioned Elastodynamics Method Based on Lagrange Multipliers

Pavel Bochev, Sandia National Laboratories, USA; Paul A. Kuberry, Clemson University, USA; Kara Peterson, Sandia National Laboratories, USA

10:25-10:45 Numerical Study of Viscoelastic Fluid-Structure Interaction

Hyesuk Lee, Clemson University, USA

Friday, March 3

MS284

Numerical Methods for Forward and Inverse Problems of Radiative Transport Equations - Part I of II

9:10 AM-10:50 AM

Room:212

For Part 2 see MS311

The computational modeling and simulation of radiative transport processes in complex media find applications in many important fields of science and technology, including, for instance, the classical application in describing neutron transport in reactors, as well as the modern application in optical imaging of heterogeneous media (such as biological tissues) with near infra-red photons. This minisymposium intends to bring in leading experts in computational transport research to discuss recent developments in the numerical solutions of forward and inverse radiative transport problems in different applications.

Organizer: Kui Ren

University of Texas at Austin, USA

Organizer: Yimin Zhong

University of Texas at Austin, USA

9:10-9:30 Curvature Correction and Corner Layer of the Transport Equation

Qin Li, University of Wisconsin, USA; Jianfeng Lu, Duke University, USA; Weiran Sun, Simon Fraser University, Canada

9:35-9:55 Title Not Available At Time Of Publication

Andreas H. Hielscher, Columbia University, USA

10:00-10:20 Void-Compatible Second-Order Forms of the Transport Equation

Ryan McClarren, Weixiong Zheng, and Vincent Laboure, Texas A&M University, USA

10:25-10:45 Title Not Available At Time Of Publication

Justin Pounders, Bettis Laboratory, USA

Friday, March 3

MS285

High-Performance Eigenvalue and SVD Solvers: Advances and Applications - Part I of II

9:10 AM-10:50 AM

Room:213

For Part 2 see MS312

This minisymposium is concerned with innovative methods and high-performance software for large scale eigenvalue and SVD computations. The increasing complexity and size of modern scientific computing simulations and machine learning applications introduce significant challenges to existing eigenvalue and SVD solvers. This minisymposium will describe efforts to increase the efficiency of algorithms and software, extensions of their usability to next generation computers, and the related practical applications.

Organizer: Lingfei Wu

IBM T.J. Watson Research Center, USA

Organizer: Andreas Stathopoulos

College of William & Mary, USA

Organizer: Eloy Romero

College of William & Mary, USA

9:10-9:30 PRIMME_SVDS: A High-Performance Preconditioned SVD Solver for Accurate Large-Scale Computations

Lingfei Wu, IBM T.J. Watson Research Center, USA; Andreas Stathopoulos and Eloy Romero, College of William & Mary, USA

9:35-9:55 Randomized Algorithm for Computing Or Updating SVD

Ichitaro Yamazaki, Jakub Kurzak, and Piotr Luszczek, University of Tennessee, USA; Jack J. Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA

10:00-10:20 Applying the Feast Sparse Eigensolver to the Singular Value Decomposition

Brendan Gavin and Eric Polizzi, University of Massachusetts, Amherst, USA

10:25-10:45 Iterative Lanczos Methods for Principal Components Analysis of Genomics Data

Jiahao Chen, Massachusetts Institute of Technology, USA

Friday, March 3

MS286

Meshless, Particle, and Particle-Mesh Methods for PDEs - Part II of II

9:10 AM-10:25 AM

Room:214

For Part 1 see MS260

Due to their inherent scalability, meshless, particle-based and particle-mesh methods are becoming increasingly important with recent increases in available computing power. Meshless and particle-based methods provide adaptive solutions for problems with deforming interfaces, without the burden of generating boundary conforming meshes. Particle and particle- mesh methods become critically important as scientific and engineering applications move towards more resolved / first principles approaches. In addition to classical applications of particle methods for PDEs in electromagnetism and cosmology, new applications in climate, energy, and environmental areas are adopting particle and hybrid methods. We focus on recent developments using these methods to scalably solve PDEs with diverse applications to scientific and engineering problems. In particular, a spectrum of methods will be represented: Lagrangian particle methods for hydrodynamic problems, recent advances in smoothed particle hydrodynamics, staggered moving least squares, PIC methods for plasma physics problems, as well as topics from scattered data approximation theory. Research issues of particular interest include rigorous foundations of methods based on mathematical approximation theory, error analysis and convergence, improved kernels and high order methods, spatial and temporal adaptivity, and scalability on modern supercomputer architectures.

Organizer: Alexandre M. Tartakovsky

Pacific Northwest National Laboratory, USA

continued on next page

Organizer: Roman Samulyak
Stony Brook University, USA

9:10-9:30 Lagrangian Particle Methods for Euler Equations: Stability, High Order Convergence, and Limiters
Roman Samulyak and Xingyu Wang, Stony Brook University, USA

9:35-9:55 Adaptive Particle-in-Cloud Method for Optimal Solutions of Vlasov-Poisson Equations
Xingyu Wang and Roman Samulyak, Stony Brook University, USA; Xiangmin Jiao, State University of New York, Stony Brook, USA; Kwangmin Yu, Brookhaven National Laboratory, USA

10:00-10:20 Scalable Mesh Infrastructure for Particle-in-Cell Magnetic Fusion Simulations
Eisung Yoon, Mark S. Shephard, Kaushik Kalyanaraman, E. Seegyoung Seol, and Dan A. Ibanez, Rensselaer Polytechnic Institute, USA

Friday, March 3

MS287

Data-Driven Modeling - Part I of II

9:10 AM-10:50 AM

Room:215

For Part 2 see MS314

Projection-based model reduction has enjoyed great success in producing high-fidelity, and in some cases optimal, reduced models that can be effectively used as surrogates in prediction, control, optimization, UQ, and many other applications. However, these methods require access to internal system dynamics (full-order operators) and thus are intrusive in nature. And, in some cases, the full-model is given as a black box and access to internal dynamics are not possible. Data-driven modeling provides a powerful alternative. The approximants are data-driven, i.e., constructed using only a form of input-output data without accessing system operators. This minisymposium will bring together researchers tackling the data-driven modeling problem in two different, but closely related frameworks, namely frequency-response data based modeling and time-domain data based modeling. The MS will cover topics including identification systems from time-domain impulse response measurements, data-based modeling for an instrumented building, sparse identification of nonlinear dynamics, and structure-preserving data-driven modeling and switched systems modeling using the frequency samples,

Organizer: Serkan Gugercin
Virginia Tech, USA

Organizer: Athanasios C. Antoulas
Rice University, USA

9:10-9:30 Data-Driven Model Reduction and the Preservation of DAE Structure
Athanasios C. Antoulas, Rice University, USA

9:35-9:55 Preserving Passivity with Data-Driven Models
Christopher A. Beattie, Virginia Tech, USA

10:00-10:20 A Comparison of Three MOR Methods for LSS: The Loewner Framework, Balanced Truncation and Optimal H2
Ion Victor Gosea, Jacobs University Bremen, Germany; Athanasios C. Antoulas, Rice University, USA

10:25-10:45 $\mathcal{H}2$-Optimal Model Approximation by Structured Time-Delay Reduced Order Models
Igor Pontes Duff, Charles Poussot-Vassal, and Cédric Seren, ONERA, France

continued in next column

Friday, March 3

MS288

Advances in Adaptive Approaches for Complex Problems on Next-generation Computers - Part I of II

9:10 AM-10:50 AM

Room:216

For Part 2 see MS315

Adaptive approaches provide a very effective way to perform reliable predictions for complex physical systems. These complex systems span multiple physics and multiple scales with complicated features such as evolving interfaces, moving and deforming objects/structures, chaotic dynamics, uncertain parameters, etc. This minisymposium will place emphasis on methods and software that explore error estimation/indication, multilevel approaches, mesh adaptation and/or high-order discretization for complex and large-scale problems (including on next generation computing platforms).

Organizer: Martin Berzins

University of Utah, USA

Organizer: Onkar Sahni

Rensselaer Polytechnic Institute, USA

9:10-9:30 Adaptive Methods in Uintah for Mesh Refinement and Resilience in Time-Dependent PDEs

Martin Berzins, Alan Humphrey, Todd Harman, Aditya Pakki, Sahithi Chaganti, and Damodar Sahasrabudhe, University of Utah, USA

9:35-9:55 The Resiliency of Multilevel Methods on Next Generation Computing Platforms: Probabilistic Model and Its Analysis

Mark Ainsworth and *Christian Glusa*, Brown University, USA

continued in next column

10:00-10:20 Towards an Exascale Hyperbolic PDE Engine: High-Order ADER-DG on Tree-Structured Cartesian Meshes

Vasco Varduhn and Jean-Matthieu Gallard, Technische Universität München, Germany; Dominic E. Charrier and Tobias Weinzierl, Durham University, United Kingdom; *Michael Bader*, Technische Universität München, Germany

10:25-10:45 Multilevel Inference with PETSc

Matthew G. Knepley, Rice University, USA; Margarete A. Jadamec, University of Houston, USA; *Tobin Issac*, University of Chicago, USA

Friday, March 3

MS290

Application and Algorithm Development using Trilinos - Part I of II

9:10 AM-10:50 AM

Room:218

For Part 2 see MS317

Upon its inception in 2000, the Trilinos project was comprised of a small number of libraries focusing on sparse linear solvers. Since then, the project scope has grown to include many other areas, such as architecture portable computation kernels, fundamental sparse linear algebra, linear and nonlinear solvers, meshing and load balancing, discretization kernels, and uncertainty quantification.The Trilinos user base is distributed among national labs, universities, and companies worldwide. The talks in these minisymposia illustrate the wide breadth of application and library research that is enabled by Trilinos capabilities. Some talks will focus on application areas, e.g., inelastic thermomechanical analysis and reduced order modeling for wind turbine wake modeling, while other talks will discuss development of scientific libraries built using Trilinos capabilities.

Organizer: Christopher Siefert

Sandia National Laboratories, USA

Organizer: Jonathan J. Hu

Sandia National Laboratories, USA

9:10-9:30 Enabling Low Mach Fluid Simulations Using Trilinos

Jonathan J. Hu, Sandia National Laboratories, USA; Andrey Prokopenko, Oak Ridge National Laboratory, USA; Mark Hoemmen, Paul Lin, Christopher Siefert, Christian Trott, and Stefan P. Domino, Sandia National Laboratories, USA

9:35-9:55 Using Trilinos Components to Construct Reduced Order Models for Wind Turbine Wake Development from Lidar Measurements

Simon Rush and Kevin Long, Texas Tech University, USA

continued on next page

10:00-10:20 Large Scale Computational Inelasticity Using the Trilinos Framework

Assad Oberai, Zhen Li, Brian Granzow, Dan A. Ibanez, Max Bloomfield, and Mark S. Shephard, Rensselaer Polytechnic Institute, USA; Glen Hansen and Christopher Siefert, Sandia National Laboratories, USA

10:25-10:45 A Parallel Approach for the Multi-Level HP-Adaptive Finite Cell Method

John Jomo, Nils Zander, Mohamed Elhaddad, Ali Oezcan, Stefan Kollmannsberger, Ralf-Peter Mundani, and Ernst Rank, Technische Universität München, Germany

Friday, March 3

MS291

Progress and Challenges in Extreme Scale Scientific Computing and Data - Part I of II

9:10 AM-10:50 AM

Room:219

For Part 2 see MS318

Extreme scale computing efforts have resulted in numerous advances for multicore, manycore and accelerator based scalable systems. In addition, large-scale simulations must increasingly deal with data management and analysis as a first-class concern. In this minisymposium we present some of the latest work in scalable algorithms and libraries for next generation computing platforms. Furthermore, we discuss efforts to better incorporate data science concerns as a principle component of our scientific workflows.

Organizer: Michael Heroux

Sandia National Laboratories, USA

Organizer: Kengo Nakajima

University of Tokyo, Japan

Organizer: Serge G. Petiton

Université Lille 1 and CNRS, France

9:10-9:30 Application Development Framework for Manycore Architectures in Post-K/Post-Moore Era

Kengo Nakajima, University of Tokyo, Japan

9:35-9:55 ShyLU: A Collection of Node-Scalable Sparse Linear Solvers

Siva Rajamanickam, Kyungjoo Kim, Andrew Bradley, and Erik G. Boman, Sandia National Laboratories, USA

10:00-10:20 CHiS: An Efficient CPU/GPU Direct Linear System Solver for 3D FDFD Photonic Device Analysis

Weichung Wang and Cheng-Han Du, National Taiwan University, Taiwan

10:25-10:45 Convergence Between Big Data and HPC from the Application Point of View

Christophe Calvin, CEA Saclay, France

Friday, March 3

MS292

Stochastic Optimization with Differential Equations: Methods and Applications - Part I of II

9:10 AM-10:50 AM

Room:220

For Part 2 see MS319

Mathematical models involving stochastic (partial) differential equations allow both for an accurate description of physical processes, and to include modeling uncertainties. Stochastic optimization in such models can be used for parameter estimation, noise filtering, uncertainty quantification, and experimental design in the presence of randomness or uncertainties. Due to high complexity of the models and uncertainties, such a process is computationally challenging. This mini-symposium brings together mathematicians and engineers to trigger discussions and exchange new ideas in this emerging field. Our talks will range from mathematical analysis through algorithmic design to the results of practical applications.

Organizer: Huanhuan Yang

Florida State University, USA

Organizer: Konstantin Pieper

Florida State University, USA

9:10-9:30 Effective Computational Methods for Optimal Control Problems of Random PDEs

Hyung-Chun Lee, Ajou University, South Korea; Max Gunzburger, Florida State University, USA

9:35-9:55 Inverse Problems Matching Statistical Moments in PDEs with Random Data

Catalin S. Trenchea, University of Pittsburgh, USA

10:00-10:20 Multi-Level Monte Carlo Finite Element Method for Stochastic Optimal Control Problem

Ju Ming, Beijing Computational Science Research Center, China; Qiang Du, Columbia University, USA; Qi Sun, Beijing Computational Science Research Center, China

10:25-10:45 Backward SDE Methods for Nonlinear Filtering Problems

Yanzhao Cao, Auburn University, USA

Friday, March 3

MS293

Uncertainty Quantification in Multi-Scale Systems - Part I of II

9:10 AM-10:50 AM

Room:Crystal AF - 1st Flo

For Part 2 see MS321

Quantifying the uncertainty in multi-scale models has becoming crtical in the modeling of systems characterized by multi-scale behaviors. Uncertainties in different scales exhibit different features, and the propagation and interaction of the uncertainties across scales can have substantial effect on the properties of the system. This minisymposium will explore recent advances in numerical algorithms and applications for uncertainty quantification in multi-scale systems including propagation of uncertainty across different scales or domains (e.g., from continuum to micro-scales), uncertainty of under-resolution simulations (e.g., climate models), and model reduction in multi-scale high-dimensional complex systems (e.g., turbulent flows).

Organizer: Xiu Yang

Pacific Northwest National Laboratory, USA

Organizer: Heng Xiao

Virginia Tech, USA

9:10-9:30 Uncertainty Quantification in the Accelerated Climate Modeling for Energy

Hui Wan, Xiu Yang, Alexandre M. Tartakovsky, Yun Qian, and Philip J. Rasch, Pacific Northwest National Laboratory, USA

9:35-9:55 A Data-Driven Approach to Quantify and Reduce Model-Form Uncertainty in Turbulent Flow Simulations

Jianxun Wang, Jinlong Wu, and Heng Xiao, Virginia Tech, USA

10:00-10:20 Optimal Regularized Inverse Matrices for Inverse Problems

Matthias Chung, Virginia Tech, USA

10:25-10:45 Efficient UQ Strategies in High-Dimensional Inverse Problems

Eric De Sturler, Virginia Tech, USA; Misha E. Kilmer, Tufts University, USA; Arvind Saibaba, North Carolina State University, USA; Eric L. Miller, Tufts University, USA

Friday, March 3

MS294

Finite Element Methods for Weather, Oceans and Climate - Part I of II

9:10 AM-10:50 AM

Room:Crystal CD - 1st Fl

For Part 2 see MS320

Finite elements, including spectral element methods, discontinuous Galerkin methods and compatible finite element methods, provide the flexibility to use non-orthogonal and pseudo-uniform meshes on the sphere, as well as unstructured meshes that can be used in multiresolution and adaptive mesh simulations and to resolve topography and coastlines in ocean models, with the ability to maintain consistency and increase the order of accuracy. Finite element methods now form the basis of a number of dynamical core research groups and ocean modelling groups. The application to oceans, weather and climate brings with it specific issues due to the large range of different time and space scales in the problem. Hence, there are many specific aspects that must be considered, examples include compatibility of discretisations with geophysical balances, timestepping algorithms and linear solvers to deal with the large aspect ratios in ocean and atmosphere shaped domains, conservation of energy, mass, momentum, potential vorticity etc., and integration with physics parameterisations. This is currently a rich and vibrant research area and this minisymposium will consider the breadth of approaches and activities in it.

Organizer: Colin J. Cotter

Imperial College, United Kingdom

Organizer: Andrew McRae

University of Bath, United Kingdom

continued in next column

9:10-9:30 A Compatible Finite Element Dynamical Core

Colin J. Cotter, Jemma Shipton, Hiroe Yamazaki, and David Ham, Imperial College, United Kingdom

9:35-9:55 High Level Implementation of Geometric Multigrid Solvers for Finite Element Problems: Applications in Atmospheric Modelling

Lawrence Mitchell, Imperial College London, United Kingdom; Eike H. Mueller, University of Bath, United Kingdom

10:00-10:20 Multirate Time Stepping for Accelerating Explicit Discontinuous Galerkin Computations with Application to Geophysical Flows

Vincent Legat, Universite Catholique de Louvain, Belgium

10:25-10:45 The Numa Framework for Nonhydrostatic Atmosphere and Ocean Modeling

Frank Giraldo, Naval Postgraduate School, USA; Michal Kopera, University of California, Santa Cruz, USA; Jeremy E. Kozdon and Daniel Abdi, Naval Postgraduate School, USA

Friday, March 3

MS295

The Modeling of Biological Soft Matter Systems in Fluids - Part I of II

9:10 AM-10:50 AM

Room:301

For Part 2 see MS322

Soft matter encompasses a wide variety of materials, particularly in the area of biology. The dynamics of these soft matter systems in fluids is complex, and advanced modeling techniques are required to gain a fundamental understanding of these systems. The purpose of this minisymposium is to bring together researchers interested in the numerical tools required to model these systems, in addition to the use of these tools to gain a qualitative and quantitative understanding of these complex systems. It is hoped that researchers investigating a wide range of scales will be available, to provide a multiscale view of these important systems.

Organizer: David Salac

State University of New York at Buffalo, USA

9:10-9:30 Soft Matter and Fluids: An Overview and Challenges

David Salac, State University of New York at Buffalo, USA

9:35-9:55 Sharp Interface Immersed Boundary Methods for Heart Valve Fluid-Structure Interaction

Boyce E. Griffith, Amneet P.S. Bhalla, and Ebrahim Kolahdouz, University of North Carolina at Chapel Hill, USA

10:00-10:20 Confining Active Matter

David Saintillan, University of California, San Diego, USA

10:25-10:45 The Role of Cytoplasmic Rheology in Blebbing Dynamics

Wanda Strychalski, Case Western Reserve University, USA; Robert D. Guy, University of California, Davis, USA

Friday, March 3

MS296

Computer Aided Clinical Trials + Surgical Planning: CSE meets Clinics - Part I of II

9:10 AM-10:50 AM

Room:302

For Part 2 see MS323

One promising frontiers of CSE is Clinics. After decades of numerical modeling oriented at understanding basic physiopathology, CSE is ready to become part of the clinical routine to support the decision-making process through Clinical Trials and Surgical Planning. This will improve significantly healthcare. It requires a strong interdisciplinary effort to integrate medical processing, scientific computing and statistics. This Minisymposium gathers scientists with different background to exchange experiences and draw perspectives of this new frontier of applied mathematics. We will focus on the integration of imaging and computational tools and the reliable prescription of boundary conditions in patient- specific modeling.

Organizer: Alessandro Veneziani

Emory University, USA

Organizer: Ajit P. Yoganathan

Georgia Institute of Technology, USA

9:10-9:30 Numerical Assessment of Hemodynamics in Retro-Fontan Connections

Camille Johnson and Zhenglun Wei, Georgia Institute of Technology, USA; Ritchie Sharon and Mahesh Kappanayil, Amrita Institute of Medical Sciences and Research Centre, India; *Ajit P. Yoganathan*, Georgia Institute of Technology, USA

9:35-9:55 Fluid-Structure Interaction in Abdominal Aortic Aneurysms: Multiscale Modeling of Tissue Mechanics and a Novel Wall Shear Stress Risk Assessment

Alessio Gizzi, University Campus Bio-medico of Rome, Italy; Daniele Bianchi and Elisabetta Monaldo, Universita' di Roma Tor Vergata, Italy; Michele Marino, Leibniz Universität Hannover, Germany; Giuseppe Vairo, Universita' di Roma Tor Vergata, Italy; Simonetta Filippi, University of Rome La Sapienza, Italy

10:00-10:20 A Framework for Data Assimilation and Identifiability Issues in Computational Hemodynamics

Jean-Frederic Gerbeau, Inria Paris-Rocquencourt, France

10:25-10:45 A Comprehensive Framework for Thoracic Aortic Endograft Simulations: from Virtual Deployment to Computational Fluid-Dynamics

Rodrigo M. Romarowski, Elena Faggiano, Michele Conti, and Simone Morganti, University of Pavia, Italy; Santi Trimarchi, IRCCS Policlinico San Donato, Italy; Ferdinando Auricchio, University of Pavia, Italy

continued in next column

Friday, March 3

MS297

Modeling and Applications with Kinetic and Transport Models - Part I of II

9:10 AM-10:50 AM

Room:303

For Part 2 see MS324

This minisymposum is focused on the role of kinetic and transport theory outside of traditional physics-based modeling applications. Recently developed models in the areas of social and economic sciences, as well as high performance computing will be presented which utilize this theoretical framework.

Organizer: Richard C. Barnard
Oak Ridge National Laboratory, USA

Organizer: Michael Herty
RWTH-Aachen, Germany

9:10-9:30 A Transport Model of Data Flows in HPC Environments

Richard C. Barnard and Cory Hauck, Oak Ridge National Laboratory, USA

9:35-9:55 Phase Transition in a Model for Gang Territorial Development

Alethea Barbaro and Abdulaziz Alsenafi, Case Western Reserve University, USA

10:00-10:20 Inhomogeneous Boltzmann-Type Equations Modelling Opinion Leadership and Political Segregation

Bertram Düring, University of Sussex, United Kingdom

10:25-10:45 Uncertainty Quantification for Kinetic Equations in Socio-Economic Sciences

Mattia Zanella, University of Ferrara, Italy

Friday, March 3

MS298

Multi-scale Modeling and Computation of Active Suspensions - Part I of II

9:10 AM-10:50 AM

Room:304

For Part 2 see MS325

Active suspensions, which can consist micro-swimmers, vesicles, microtubule-motor networks or other types of active particles immersed in liquid, exhibit complex dynamics and patterns. Capturing the interplays between the particles and the surrounding fluid in continuum or agent-based models presents significant challenges as hydrodynamic interactions happen on short and long scales. Added difficulties arise when such suspensions interact with boundaries, and peculiar behavior has been observed in experiments mimicking the suspensions' natural habitats. This minisymposium's goal is to explore recent advances, especially on the computational front, on this emerging and expanding topic.

Organizer: Enkeleida Lushi
Brown University, USA

Organizer: Tong Gao
Michigan State University, USA

9:10-9:30 Individual and Collective Dynamics of Bacteria and Micro-Algae in Confinement

Enkeleida Lushi, Brown University, USA

9:35-9:55 Geometry-Dependent Viscosity Reduction in Sheared Active Fluids

Jorn Dunkel and Jonasz Slomka, Massachusetts Institute of Technology, USA

10:00-10:20 Structure and Dynamics of Dense Active Suspension Under Confinement

Tong Gao, Michigan State University, USA

10:25-10:45 Transitions to Spontaneous Flows in Confined Active Suspensions

David Saintillan, University of California, San Diego, USA

Friday, March 3

MS299

Bayesian Optimal Experimental Design for ODE/PDE Models - Part I of II

9:10 AM-10:50 AM

Room:305

For Part 2 see MS326

The challenge of optimal information gathering---for the purpose of inference, prediction, design, or control---pervades fields ranging from geophysics to chemical engineering and beyond. These questions can be formalized through the framework of optimal experimental design. Yet extending classical design methodologies to tackle problems of greater scale and dynamic complexity, and to find optimal sequential designs, requires new algorithms and formulations. This minisymposium will gather a wide variety of approaches focusing on design for large-scale inverse problems and nonlinear models, design in the presence of model error, and the approximation and optimization of information metrics. Relevant techniques include surrogate modeling, model reduction, sparse quadrature, asymptotic approximations, PDE/ODE-constrained optimization, stochastic optimization, transport maps, and approximate dynamic programming. We invite contributions focused on methodology and motivated by engineering and science applications.

Organizer: Xun Huan
Sandia National Laboratories, USA

Organizer: Omar Ghattas
University of Texas at Austin, USA

Organizer: Youssef M. Marzouk
Massachusetts Institute of Technology, USA

continued on next page

9:10-9:30 Challenges in Computing Bayesian Designs for Complex Models
David Woods and Yiolanda Englezou, University of Southampton, United Kingdom; Tim Waite, University of Manchester, United Kingdom

9:35-9:55 Approximate Experimental Design in High Dimensional Spaces
Xiao Lin and Gabriel Terejanu, University of South Carolina, USA

10:00-10:20 Adjoint-Based Methods for Design of Optimal Experiments for PDE Models
Ekaterina Kostina and Gregor Kriwet, Universität Heidelberg, Germany

10:25-10:45 Scalable Methods for Optimal Experimental Design for Inverse Scattering
Jeonghun Lee, Umberto Villa, Peng Chen, and Omar Ghattas, University of Texas at Austin, USA

Friday, March 3

MS300

Using Protein Folding to Introduce Students to Computational Sciences

9:10 AM-10:50 AM

Room:221

Protein structure prediction remains a grand challenge in modern science. Scoring the large number of protein models generated by methods that take advantage of High-Performance Computing (HPC) is a main bottleneck. Machine learning offers great promise to clear this bottleneck, situating the problem at the intersection of biology, data science, statistics, and HPC. For a period of 9 weeks, the WeFold project that brings together researchers worldwide to collaborate on protein folding becomes an educational framework to expose students and faculty to multidisciplinary research. This symposium features speakers from the 2016 experience, which focused on applying machine learning techniques to improve the current state of the art in protein scoring functions. The steep learning curve and the impressive results suggest that this approach is effective to introduce students to computational sciences and HPC and to increase diversity in these fields.

Organizer: Silvia N. Crivelli
Lawrence Berkeley National Laboratory and University of California, Davis, USA

9:10-9:30 Protein Structure Scoring Using Kernel Ridge Regression and Support Vector Machine
Itzhel Dimas, Austin Chung, and Shokoufeh Mirzaei, California Polytechnic State University, Pomona, USA

9:35-9:55 Experiments in Protein Folding Research Using a Highly Dynamic and Extendable Computational Framework
James R. Inscoe and Bogdan Czejdo, Fayetteville State University, USA; Silvia N. Crivelli, Lawrence Berkeley National Laboratory and University of California, Davis, USA

continued in next column

10:00-10:20 Using HPC to Calculate Features for Millions of Protein Models
Babatunde Adetoro, Mountain View Community College, USA; Juan Sosa, University of Texas at Dallas, USA; Jesse Fox, Mountain View Community College, USA

10:25-10:45 Machine Learning Methods for Pairwise Scoring of Protein Models
Conrad Czejdo, University of North Carolina at Chapel Hill, USA; Silvia N. Crivelli, Lawrence Berkeley National Laboratory and University of California, Davis, USA

Friday, March 3

CP21

Simulation and Modeling

9:10 AM-10:50 AM

Room:223

Chair: To Be Determined

9:10-9:20 A Partition of Unity Method for Generalized Eigenvalue Problems with Applications in Electronic Structure Calculations

Marc A. Schweitzer, Universität Bonn, Germany; Constanze Klaar and Albert Ziegenhagel, Fraunhofer SCAI, Germany

9:22-9:32 A Parallel Approach to Viscoelastic Polymer Gel Modeling

Erik Palmer, University of South Carolina, USA

9:34-9:44 Arbitrary-Shaped Walls with Controllable Surface Roughness in Dissipative Particle Dynamics Simulations

Zhen Li, Brown University, USA; Xin Bian, Technische Universität München, Germany; Yu-Hang Tang and George E. Karniadakis, Brown University, USA

9:46-9:56 An Adaptive Coupled Level Set and Moment-of-Fluid Method for Simulating the Solidification Process in Multimaterial Systems

Mehdi Vahab, University of California, Davis, USA; Mark Sussman and M. Yousuff Hussaini, Florida State University, USA

9:58-10:08 Analysis of DMA Instrumentation for Viscoelastic Materials Using the DPG Methodology

Federico Fuentes, Leszek Demkowicz, and Aleta Wilder, University of Texas at Austin, USA

10:10-10:20 Improving the Computational Efficiency of Multiscale Simulations with Filtering

David J. Gardner, Lawrence Livermore National Laboratory, USA; Daniel R. Reynolds, Southern Methodist University, USA

10:22-10:32 Risk Analysis Using Monte Carlo Simulation in Bowtie Models

Ionut E. Iacob, Georgia Southern University, USA

Friday, March 3

CP22

Computational Science - Part I of II

9:10 AM-10:50 AM

Room:224

For Part 2 see CP23

Chair: To Be Determined

9:10-9:20 Simd-Acceleration of a Sparse Analytical Chemical Kinetic Jacobian Code Via Python

Nicholas Curtis, University of Connecticut, USA

9:22-9:32 Adding Plasticity to the Oof Finite-Element Solver for Materials Science

Andrew Reid, National Institute of Standards and Technology, USA; Shahriyar Keshavarz, Theiss Research, USA; Stephen Langer, National Institute of Standards and Technology, USA

9:34-9:44 A Fast Treecode Algorithm for Stokes Flow in 3D

Lei Wang, University of Wisconsin, Milwaukee, USA; Robert Krasny, University of Michigan, Ann Arbor, USA; Svetlana Tlupova, Farmingdale State College, USA

9:46-9:56 A Quadratic High-Order Method for Mesh Generation Inspired by LBWARP

Mike Stees and Suzanne M. Shontz, University of Kansas, USA

9:58-10:08 Porting a Real-World Molecular Dynamics Application to Xeon Phi Coprocessors

Yang Yang and Aiqing Zhang, Institute of Applied Physics and Computational Mathematics, China; Letian Kang, Hunan University, China; Han Wang, CAEP Software Center for Numerical Simulation, China; Wenjie Hong, Hunan University, China

10:10-10:20 Saving Time and Energy with Oversubscription in Ab Initio Calculations for Large Chemical Systems

Masha Sosonkina, Ames Laboratory, USA; Ellie Fought, Iowa State University, USA; Vaibhav Sundiyal, Old Dominion University, USA; Theresa Windus, Iowa State University, USA

continued in next column

10:22-10:32 Hybrid Computing In Large-Scale Multiphysics Simulation: Tabulated Properties & Particle-Cell Interpolations

Babak Goshayeshi, Tony Saad, and James C. Sutherland, University of Utah, USA

10:34-10:44 A Graphical Programming Approach for Parallel Particle Based Simulation Development

Li Liao and First Name Jing, Institute of Applied Physics and Computational Mathematics, China

Coffee Break

10:50 AM-11:20 AM

Room:Foyer - 2nd Fl

Friday, March 3

MS225

Optimization Methods and Parallel Computing for Tensor Problems - Part II of II

11:20 AM-1:00 PM

Room:222

For Part 1 see MS199

Tensor (or higher-order matrix) naturally arises in applications that collect data along multiple dimensions (also called mode or way) such as in neuroimaging, multivariate statistics, multilinear algebra, data mining, speech recognition, to name a few. Since multi-way data can easily require terabytes, this makes it a great challenge for computation, data storage and transfer. Towards finding solutions of tensor problems efficiently, exploration of structures of the data, designing specific optimization methods, and also utilizing modern high-performance parallel computers are much needed. The two sessions will have recent developments along these lines.

Organizer: Yangyang Xu

University of Alabama, USA

Organizer: Carmeliza Navasca

University of Alabama at Birmingham, USA

11:20-11:40 Decomposition and Rank Approximation for Symmetric Tensors

Carmeliza Navasca, University of Alabama at Birmingham, USA

11:45-12:05 Generating Polynomials and Symmetric Tensor Decompositions

Jiawang Nie, University of California, San Diego, USA

12:10-12:30 Semialgebraic Geometry of Nonnegative Tensor Rank

Yang Qi, Gipsa-Lab, France

12:35-12:55 Leveraging Linear Constraints when Decomposing Large-scale, Incomplete Tensors

Nico Vervliet, Otto Debals, and Lieven De Lathauwer, KU Leuven, Belgium

Friday, March 3

MS301

Highly Scalable Solvers for Computational PDEs - Part II of II

11:20 AM-1:00 PM

Room:Grand Ballroom - 2nd Fl

For Part 1 see MS274

Efficient computational solution of high fidelity large-scale problems in computational science and engineering is still a major challenge. Complex applications include difficulties such as transient problems with widely varying time and spatial scales, strongly coupled multiphysics, heterogenous media, nonlinearlities, etc. The development of efficient linear system solvers for these classes of problems has many challenges, especially for high fidelity large-scale simulations, which makes proper preconditioning critical. This minisymposium will focus on highly scalable preconditioners, for example multigrid or domain decomposition approaches, multiphysics solvers (e.g. based on block factorization techniques), nonlinear preconditioning, multiscale solvers for heterogenous problems or space-time solvers, etc.

Organizer: Santiago Badia

Universitat Politecnica de Catalunya, Spain

Organizer: Paul Lin

Sandia National Laboratories, USA

11:20-11:40 A Performance Study of the Use of GPUs in Hypre

Ulrike Meier Yang, Lawrence Livermore National Laboratory, USA

11:45-12:05 A Highly Scalable Implementation of the BDDC Preconditioner

Alberto Martin, International Center for Numerical Methods in Engineering, Spain; Santiago Badia and Javier Principe, Universitat Politecnica de Catalunya, Spain

12:10-12:30 Scalable Spectral-Geometric-Algebraic Multigrid and Schur Complement Preconditioning for Nonlinear, Multiscale, Heterogeneous Flow in Earth's Mantle

Johann Rudi, University of Texas at Austin, USA; Georg Stadler, Courant Institute of Mathematical Sciences, New York University, USA; A. Cristiano I. Malossi, IBM Research-Zurich, Switzerland; Tobin Isaac, University of Chicago, USA; Michael Gurnis, California Institute of Technology, USA; Peter W. J. Staar, Yves Ineichen, Costas Bekas, and Alessandro Curioni, IBM Research-Zurich, Switzerland; Omar Ghattas, University of Texas at Austin, USA

12:35-12:55 Performance of Scalable AMG-based Preconditioners for MHD and Multifluid Plasma Simulations

Paul Lin, John Shadid, Edward G. Phillips, and Jonathan J. Hu, Sandia National Laboratories, USA; Andrey Prokopenko, Oak Ridge National Laboratory, USA; Paul Tsuji, Lawrence Livermore National Laboratory, USA; Eric C. Cyr and Roger Pawlowski, Sandia National Laboratories, USA

continued in next column

Friday, March 3

MS302

Reduced Models and Multiscale Methods - Part II of II

11:20 AM-1:00 PM

Room:Ballroom D - 2nd Fl

For Part 1 see MS275

Accurate and efficient simulations of physical responses in large-scale heterogeneous media is crucial to search and image geological formations in a wide range of geophysical applications, including mineral and hydrocarbon exploration, water resource utilizations, and geothermal power extractions. One major challenge in practice to perform this type of simulations is the excessive computational cost it involves. In this session we explore ways to reduce the complexity and the cost of the simulation by introducing multiscale and upscaling methods as well as reduce space modeling.

Organizer: Luz Angelica Caudillo Mata

University of British Columbia, Canada

Organizer: Eldad Haber

University of British Columbia, Canada

11:20-11:40 A Multiscale Mimetic Method for Maxwell's Equations

Eldad Haber, University of British Columbia, Canada

11:45-12:05 PDE-Constrained Optimization with Multiscale Methods

Samy Wu Fung and Lars Ruthotto, Emory University, USA; Eldad Haber, University of British Columbia, Canada

12:10-12:30 Tensor T-Product Model Reduction

Jiani Zhang, Tufts University, USA; Lior Horesh, IBM Research, USA; Haim Avron, Tel Aviv University, Israel; Misha E. Kilmer, Tufts University, USA

12:35-12:55 A General, Efficient and Self-Correcting Enrichment Strategy for Multiscale Methods in Reservoir Simulation

Abdulrahman M. Manea, Stanford University, USA; Hadi Hajibeygi, Technical University of Delft, Netherlands; Panayot Vassilevski, Lawrence Livermore National Laboratory, USA; Hamdi Tchelepi, Stanford University, USA

Friday, March 3

MS303

Poroelasticity: Recent Theoretical and Computational Advances - Part II of II

11:20 AM-1:00 PM

Room:202

For Part 1 see MS276

Poroelasticity is the science of fluid-saturated, elastic, porous media (elastic solids) and the interactions between the fluid and the elastic porous structures. The equations of poroelasticity arise in diverse areas of science and technology, from geomechanics and geophysics to man made materials and biological tissue. Speakers will describe recent advances in the theoretical analysis and numerical approximation of solutions of the equations of poroelasticity and the analysis and simulation of related physical phenomena and the equations describing them.

Organizer: Yanzhao Cao

Auburn University, USA

Organizer: Amnon J. Meir

Southern Methodist University, USA

11:20-11:40 Analysis and Numerical Approximation of Nonlinear Poroelasticty

Amnon J. Meir, Southern Methodist University, USA

11:45-12:05 Finite Element Approximation of Nonlinear Poroelasticity

Song Chen, University of Wisconsin, La Crosse, USA

12:10-12:30 Efficient Numerical Method for Fluid Flows in Poroelastic Media

Xiaobing H. Feng, University of Tennessee, USA

12:35-12:55 A Lagrange Multiplier Method for a Stokes-Biot Model of Flow in Fractured Poroelastic Media

Ilona Ambartsumyan and Eldar Khattatov, University of Pittsburgh, USA; Paolo Zunino, Politecnico di Milano, Italy; Ivan Yotov, University of Pittsburgh, USA

Friday, March 3

MS304

Numerical Methods for Wave Propagation and Its Applications - Part II of II

11:20 AM-1:00 PM

Room:203

For Part 1 see MS277

Fast and robust numerical methods for wave propagation play a key role in lots of problems with important applications, ranging from nano-optics to medical imaging. This minisymposium will discuss recent advances in the development of fast numerical algorithms for wave equations, as well as its applications in inverse problems and optimal design, creating the opportunity for collaboration between computational mathematics and other fields, such as optics, materials sciences, and imaging sciences.

Organizer: Min Hyung Cho

University of Massachusetts, Lowell, USA

Organizer: Jun Lai

Courant Institute of Mathematical Sciences, New York University, USA

Organizer: Carlos Borges

University of Texas at Austin, USA

11:20-11:40 Simulating Surface Plasmons on Periodic Gratings Coated with Graphene: A High Order Perturbation of Surfaces Approach

David P. Nicholls, University of Illinois, Chicago, USA

11:45-12:05 A Tensor Train Acceleration for the ICVSIE for 3D High-Contrast Scatterers

Eduardo Corona, University of Michigan, USA

12:10-12:30 Robust Integral Formulations for Electromagnetic Scattering from Three-Dimensional Cavities

Jun Lai and Leslie Greengard, Courant Institute of Mathematical Sciences, New York University, USA; Michael O'Neil, New York University, USA

12:35-12:55 Wave-Structure Interaction Problems with a Piezoelastic Solid

Thomas S. Brown, University of Delaware, USA; Tonatiuh Sanchez-Vizuet, New York University, USA; Francisco J. Sayas, University of Delaware, USA

Friday, March 3

MS305

Programming Scientific Codes on Recent Multicore and Manycore Processors - Part II of II

11:20 AM-1:00 PM

Room:204

For Part 1 see MS278

Efficient computation using multiple cores continues to be a challenge, especially as new manycore architectures enter the field, such as Intel Xeon Phi Knights Landing and the ShenWei processors used in TaihuLight. The speakers will demonstrate how to achieve high performance on different applications and platforms, including scheduling and balancing multiple threads on irregular workloads, paying attention to cache and memory in the context of large numbers of concurrent threads, and exploiting features of the processors such as special memory and vectorization.

Organizer: Edmond Chow

Georgia Institute of Technology, USA

Organizer: Xiaoye Sherry Li

Lawrence Berkeley National Laboratory, USA

11:20-11:40 Opportunities and Challenges in Sparse Linear Algebra on Many-Core Processors with High-Bandwidth Memory

Jongsoo Park, Intel Corporation, USA

11:45-12:05 Exploiting Modern Manycore Architecture in Sparse Direct Solver with Runtime Systems

Pierre Ramet, Mathieu Faverge, and Gregoire Pichon, Université de Bordeaux, Inria, LaBRI, France

continued in next column

12:10-12:30 Optimizing the Earthquake Simulation Code SeisSol for Heterogeneous Xeon Phi Supercomputers

Leonhard Rannabauer, Sebastian Rettenberger, Carsten Uphoff, and Michael Bader, Technische Universität München, Germany

12:35-12:55 Refactoring Atmospheric Models on Sunway TaihuLight Many-Core Supercomputer

Wei Xue and Haohuan Fu, Tsinghua University, China; Chao Yang, Chinese Academy of Sciences, China; Lanning Wang, Beijing Normal University, China; Dexun Chen, National Research Center of Parallel Computer Engineering & Technology and Tsinghua University, China

Friday, March 3

MS306

Recent Advances in Unstructured Mesh Algorithms and Their Applications - Part II of II

11:20 AM-1:00 PM

Room:205

For Part 1 see MS279

Unstructured meshes continue to be ubiquitous in computational science and engineering simulations. In recent years, there have been some exciting developments in regards to unstructured mesh algorithms. For example, progress has been made in the areas of parallel mesh generation, high-order mesh generation, anisotropic adaptive meshing, and dynamic meshing to name just a few. Similarly, meshes have been employed in challenging simulations involving applications of fluid and solid mechanics, patient-specific medicine, design of materials, and computer graphics, and many others. The minisymposium will feature presentations on such algorithms and applications, as well as other related problems.

Organizer: Maurin A. Lopez Varilla

University of Kansas, USA

Organizer: Suzanne M. Shontz

University of Kansas, USA

11:20-11:40 A Parallel Algorithm for Variational Mesh Quality Improvement Method

Maurin A. Lopez Varilla, Suzanne M. Shontz, and Weizhang Huang, University of Kansas, USA

11:45-12:05 Parallel Geometry and Meshing Adaptation with Application to Problems with Evolving Domains

Saurabh Tendulkar, Ottmar Klaas, and Mark Beall, Simmetrix, Inc., USA; Mario Juha and Mark S. Shephard, Rensselaer Polytechnic Institute, USA

12:10-12:30 A Unified Finite Element Method for Fluid-Structure Interaction

Yongxing Wang, *Peter K. Jimack*, and Mark A. Walkley, University of Leeds, United Kingdom

12:35-12:55 Advances in Grid-Based All-Hex Mesh Generation for High Performance Computing

Steve J. Owen, Sandia National Laboratories, USA

Friday, March 3

MS307

Numerical Methods for Electronic Structure Calculations: Ground State Properties - Part II of II

11:20 AM-1:00 PM

Room:206

For Part 1 see MS280

The goal of this minisymposium is to bring experts working on numerical methods for electronic structure computations for materials together. In a wide range of applications, materials have to be studied at the quantum level. Among them, let us mention for instance conducting, magnetic or optical properties. The computation and characterization of the electronic structure of such materials raise numerous challenges from the mathematical and computational point of view, in particular due to the increasing complexity of the systems that are of interest to materials scientists. This minisymposium will focus more specifically on numerical methods for ground state calculations. The first talk of the session will give an introduction to ground state electronic structure computations and the other invited speakers will present their latest developments in the field.

Organizer: Virginie Ehrlacher

CERMICS, France

11:20-11:40 A Posteriori Error Estimation for Nonlinear Schrödinger Equations

Eric Cances, Ecole des Ponts and Inria, France; *Geneviève Dusson* and Yvon Maday, Université Pierre et Marie Curie, France; Benjamin Stamm, RWTH Aachen, Germany; Martin Vohralik, Universite de Paris VI, France

continued in next column

11:45-12:05 Robust Computation of Wannier Functions

Antoine Levitt, Inria and Ecole des Ponts ParisTech, France; Eric Cances, Ecole des Ponts and Inria, France; Gabriel Stoltz, École des Ponts ParisTech, France; Gianluca Panati, Università di Roma "La Sapienza", Italy

12:10-12:30 Second-Order Optimization of the Casscf Wavefunction in a Relativistic Framework

Filippo Lipparini and Jürgen Gauss, Johannes Gutenberg-Universität, Mainz, Germany

12:35-12:55 Locality of Electronic Structure Models

Faizan Nazar, University of Warwick, United Kingdom

Friday, March 3

MS308

Sensitivity Analysis and Uncertainty Quantification of Chaotic Systems - Part II of II

11:20 AM-12:35 PM

Room:209

For Part 1 see MS281

Chaotic dynamics appears in many scientific and engineering applications. Sensitivity analysis in the presence of chaos is challenging, but necessary to understand and control solution responses to variations in geometry, simulation parameters, and numerical discretization. Uncertainty quantification is needed to assess the accuracy and reliability of quantities predicted by chaotic dynamics simulations.

Organizer: Boris Diskin

National Institute of Aerospace, USA

Organizer: Eric Nielsen

NASA Langley Research Center, USA

11:20-11:40 Scaling of Lyapunov Exponents in Homogeneous, Isotropic Turbulence

Prakash Mohan and Robert D. Moser, University of Texas at Austin, USA

11:45-12:05 Controlling Electroconvection with Surface Patterning

Scott Davidson and Ali Mani, Stanford University, USA

12:10-12:30 Numerically Computing the Sensitivity Derivatives for Chaotic High Fidelity Simulation

Guowei He, Chinese Academy of Sciences, China

Friday, March 3

MS309

Advances in Fast Solution of Sparse and Structured Linear Systems - Part II of II

11:20 AM-1:00 PM

Room:210

For Part 1 see MS282

This minisymposium concerns the numerical solution of sparse and structured linear systems. We provide an overview of recent advances in the field, spanning preconditioned iterative methods in parallel and sequential settings, matrix equations, innovative preconditioning approaches for partial differential equations, error bounds, and Krylov subspace iterative methods for saddle point systems.

Organizer: Jessica Bosch

University of British Columbia, Canada

Organizer: Chen Greif

University of British Columbia, Canada

11:20-11:40 Fast Iterative Solvers for Cahn-Hilliard Problems

Jessica Bosch, University of British Columbia, Canada; Martin Stoll, Max Planck Institute, Magdeburg, Germany

11:45-12:05 Efficient Solvers for Stochastic Galerkin Linear Systems

Akwum Onwunta, Max Planck Institute, Magdeburg, Germany; Sergey Dolgov, University of Bath, United Kingdom; Martin Stoll, Max Planck Institute, Magdeburg, Germany; Peter Benner, Max Planck Institute for Dynamics of Complex Technical Systems, Germany

12:10-12:30 Asynchronous Optimized Schwarz Methods for the Solution of PDEs

Daniel B. Szyld, Temple University, USA; Frédéric Magoulès and Cédric Venet, CentraleSupelec and Université Paris-Saclay, France

12:35-12:55 Robust and Fast Preconcitioners for Porous Media Flow

Kees Vuik, Gabriela Diaz, and Jan Dirk Jansen, Technische Universität Delft, Germany

Friday, March 3

MS310

Coupling Strategies for PDEs - Part II of II

11:20 AM-1:00 PM

Room:211

For Part 1 see MS283

Interfaces may occur naturally when modeling physical systems in contact, or may occur artificially when used to capture material defects and small scale features in certain portions of the domain. Artificial interfaces can additionally occur when decomposing a domain to reduce computational load on each processor or when dealing with meshes for subdomains that have been generated independently. There exist a wide variety of codes for performing computational simulations of physical systems governed by partial differential equations, each having their own unique capabilities and strengths. Coupling algorithms for interfaces permit the most appropriate tool to be used dependent upon mesh and constitutive equation for each subdomain. This minisymposium aims to present research related to interface coupling methods including theoretical formulations and results from applications.

Organizer: Paul Kuberry

Sandia National Laboratories, USA

Organizer: Kara Peterson

Sandia National Laboratories, USA

11:20-11:40 An Explicit Mortar Flux Recovery Approach for Interface Coupling

Kara Peterson, Pavel Bochev, and Paul Kuberry, Sandia National Laboratories, USA

11:45-12:05 A Generalized Approach For Coupling Elliptic Problems With Material Discontinuities with Spatially Noncoincident Interfaces Through Linear Extensions

James Cheung, Florida State University, USA

12:10-12:30 Inf-Sup Stability of Geometrically Unfitted Stokes Finite Elements

Johnny Guzman, Brown University, USA; Maxim A. Olshanskii, University of Houston, USA

12:35-12:55 Concurrent Multiscale Coupling in Solid Mechanics via the Schwarz Alternating Method

Irina K. Tezaur, Alejandro Mota, and Coleman Alleman, Sandia National Laboratories, USA

Friday, March 3

MS311

Numerical Methods for Forward and Inverse Problems of Radiative Transport Equations - Part II of II

11:20 AM-1:00 PM

Room:212

For Part 1 see MS284

The computational modeling and simulation of radiative transport processes in complex media find applications in many important fields of science and technology, including, for instance, the classical application in describing neutron transport in reactors, as well as the modern application in optical imaging of heterogeneous media (such as biological tissues) with near infra-red photons. This minisymposium intends to bring in leading experts in computational transport research to discuss recent developments in the numerical solutions of forward and inverse radiative transport problems in different applications.

Organizer: Kui Ren

University of Texas at Austin, USA

Organizer: Yimin Zhong

University of Texas at Austin, USA

11:20-11:40 Inverse Transport and Acousto-Optic Imaging

John Schotland, University of Michigan, USA

11:45-12:05 Uncertainty Quantification for Multiscale Transport Equations

Shi Jin, Shanghai Jiao Tong University, China, and the University of Wisconsin-Madison, USA

12:10-12:30 Preconditioning the Discrete Ordinate Equations in Optically Thick Media

Rongting Zhang, Yimin Zhong, and Kui Ren, University of Texas at Austin, USA

12:35-12:55 Title Not Available At Time Of Publication

Guangwei Yuan, Institute of Applied Physics and Computational Mathematics, China

Friday, March 3

MS312

High-Performance Eigenvalue and SVD solvers: Advances and Applications - Part II of II

11:20 AM-1:00 PM

Room:213

For Part 1 see MS285

This minisymposium is concerned with innovative methods and high-performance software for large scale eigenvalue and SVD computations. The increasing complexity and size of modern scientific computing simulations and machine learning applications introduce significant challenges to existing eigenvalue and SVD solvers. This minisymposium will describe efforts to increase the efficiency of algorithms and software, extensions of their usability to next generation computers, and the related practical applications.

Organizer: Lingfei Wu

IBM T.J. Watson Research Center, USA

Organizer: Andreas Stathopoulos

College of William & Mary, USA

Organizer: Eloy Romero

College of William & Mary, USA

11:20-11:40 Fast Computation of Spectral Projectors of Banded Matrices

Ana Susnjara and Daniel Kressner, École Polytechnique Fédérale de Lausanne, Switzerland

11:45-12:05 Accelerating Nuclear Configuration Interaction Calculations through a Preconditioned Block Iterative Eigensolver

Meiyue Shao, Lawrence Berkeley National Laboratory, USA; H. Metin Aktulga, Michigan State University, USA; Chao Yang and Esmond G. Ng, Lawrence Berkeley National Laboratory, USA; Pieter Maris and James Vary, Iowa State University, USA

12:10-12:30 QCD with Eigenvectors

Chulwoo Jung, Brookhaven National Laboratory, USA

12:35-12:55 Domain Decomposition Approaches for Accelerating Contour Integration Eigenvalue Solvers for Symmetric Eigenvalue Problems

Vassilis Kalantzis, University of Minnesota, USA

Friday, March 3

MS313

Model and Solution Reduction Methods in Computational Mechanics: Challenges and Perspectives

11:20 AM-1:00 PM

Room:214

As numerical modeling establishes as a tool for design and optimization in many fields of science, computational effectiveness becomes mandatory. The trade-off between accuracy and efficiency is fundamental for practical applications, new generation hardware is not always the solution. Innovative numerical methods are of fundamental importance. Different approaches rely on (1) specific problem-dependent features, (2) on online/offline paradigms with a smart use of precomputed high-fidelity solutions. This minisymposium gathers scientists from different fields of computational mechanics to take advantage of several complementary experiences and perspectives toward the development of more effective solution and model reduction techniques. Supported by NSF.

Organizer: Alessandro Veneziani

Emory University, USA

Organizer: Simona Perotto

Politecnico di Milano, Italy

11:20-11:40 Hierarchical Model Reduction: Theory and Practice

Simona Perotto, Politecnico di Milano, Italy

11:45-12:05 Perspectives and Advances in Reduced Order Methods for Parametrized Viscous Flows

Gianluigi Rozza, Francesco Ballarin, and Giovanni Stabile, SISSA-ISAS International School for Advanced Studies, Italy

12:10-12:30 Reduced Basis Element for Solid Mechanics: Nitsche-Based Reduced Basis Element

Davide Baroli, University of Luxembourg, Luxembourg

12:35-12:55 Patient-Specific Blood Flow Simulations at Reduced Computational Cost: The Transversally Enriched Pipe Element Methodology (TEPEM)

Alonso M. Alvarez, Pablo Blanco, and Raúl A. Feijóo, Laboratorio Nacional de Computacao Cientifica, Brazil

Friday, March 3

MS314

Data-Driven Modeling - Part II of II

11:20 AM-1:00 PM

Room:215

For Part 1 see MS287

Projection-based model reduction has enjoyed great success in producing high-fidelity, and in some cases optimal, reduced models that can be effectively used as surrogates in prediction, control, optimization, UQ, and many other applications. However, these methods require access to internal system dynamics (full-order operators) and thus are intrusive in nature. And, in some cases, the full-model is given as a black box and access to internal dynamics are not possible. Data-driven modeling provides a powerful alternative. The approximants are data-driven, i.e., constructed using only a form of input-output data without accessing system operators. This minisymposium will bring together researchers tackling the data-driven modeling problem in two different, but closely related frameworks, namely frequency-response data based modeling and time-domain data based modeling. The MS will cover topics including identification systems from time-domain impulse response measurements, data-based modeling for an instrumented building, sparse identification of nonlinear dynamics, and structure-preserving data-driven modeling and switched systems modeling using the frequency samples,

Organizer: Serkan Gugercin

Virginia Tech, USA

Organizer: Athanasios C. Antoulas

Rice University, USA

continued on next page

11:20-11:40 Interpolatory Decompositions in an Instrumented Building

Mark Embree, Virginia Tech, USA; Dustin Bales, GAiTE, LLC, USA; Serkan Gugercin and Pablo Tarazaga, Virginia Tech, USA

11:45-12:05 Discovering Governing Equations by Sparse Identification of Nonlinear Dynamics

Steven Brunton, University of Washington, USA; Joshua L. Proctor, Institute for Disease Modeling, USA; Nathan Kutz, University of Washington, USA

12:10-12:30 Fast Data-Driven System Identification from Impulse Response Measurements

Jeffrey M. Hokanson, Colorado School of Mines, USA

12:35-12:55 Data-Driven Model Order Reduction for Linear Parametric Systems

Yao Yue, Max Planck Institute for Dynamics of Complex Technical Systems, Germany; Lihong Feng, Max Planck Institute, Magdeburg, Germany; Peter Benner, Max Planck Institute for Dynamics of Complex Technical Systems, Germany

Friday, March 3

MS315

Advances in Adaptive Approaches for Complex Problems on Next-generation Computers - Part II of II

11:20 AM-1:00 PM

Room:216

For Part 1 see MS288

Adaptive approaches provide a very effective way to perform reliable predictions for complex physical systems. These complex systems span multiple physics and multiple scales with complicated features such as evolving interfaces, moving and deforming objects/ structures, chaotic dynamics, uncertain parameters, etc. This minisymposium will place emphasis on methods and software that explore error estimation/indication, multilevel approaches, mesh adaptation and/or high-order discretization for complex and large-scale problems (including on next generation computing platforms).

Organizer: Martin Berzins

University of Utah, USA

Organizer: Onkar Sahni

Rensselaer Polytechnic Institute, USA

11:20-11:40 Mesh Motion and Adaptation for Two-Phase Flow Problems with Moving Objects

Onkar Sahni, Alvin Zhang, and Mark S. Shephard, Rensselaer Polytechnic Institute, USA; Chris Kees, U.S. Army Engineer Research and Development Center, USA

11:45-12:05 Adaptivity in High-Order Finite Element ALE Simulations

Jakub Cerveny, Veselin Dobrev, *Tzanio V. Kolev*, Robert Rieben, and Vladimir Tomov, Lawrence Livermore National Laboratory, USA

12:10-12:30 Parallel Goal-Oriented Adaptive Solid Mechanics

Brian Granzow, Assad Oberai, and Mark S. Shephard, Rensselaer Polytechnic Institute, USA

12:35-12:55 Modeling Laser Absorption in Low-Speed Reacting Flows using Adaptive Finite Elements

Timothy Adowski and Paul Baumann, State University of New York at Buffalo, USA

Friday, March 3

MS316

Advances in Linear Scaling Algorithms for Electronics Structure Calculations

11:20 AM-1:00 PM

Room:217

Electronic structure calculations based on density functional theory requires the solution of a nonlinear eigenvalue problem that can be challenging to solve. Traditional solution strategies such as those based on plane-waves basis have been favored in the physics community due to their sound theoretical foundation and well established accuracy. However, the computational cost of these traditional algorithms scales as $O(N^3)$ with an $O(N^2)$ storage complexity for the solution. This limits the size of problems that can be solved and hinders the efficient use of HPC resources. This minisyposium addresses recent advances in the development of linear scaling algorithms including exploiting existing and emerging advancements in HPC resource architectures; and the development of state-of-the-art numerical strategies to improve the accuracy and stability of $O(N)$ algorithms, to enable the simulation of larger and realistic applications. We bring together application scientists, mathematicians, and computer scientists who are adapting and advancing research in linear scaling algorithms for electronics structure calculations.

Organizer: Daniel Osei-Kuffuor

Lawrence Livermore National Laboratory, USA

Organizer: Jean-Luc Fattebert

Lawrence Livermore National Laboratory, USA

11:20-11:40 O(N) Density Functional Theory Calculations: Beyond Ground State of Insulators

Jean-Luc Fattebert, Daniel Osei-Kuffuor, and Tadashi Ogitsu, Lawrence Livermore National Laboratory, USA

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Friday, March 3

MS316

Advances in Linear Scaling Algorithms for Electronics Structure Calculations

11:20 AM-1:00 PM

continued

11:45-12:05 Spectral Quadrature Method for Large-Scale, High-Temperature Quantum Molecular Dynamics

Phanish Suryanarayana, California Institute of Technology, USA

12:10-12:30 Next Generation Quantum Molecular Dynamics

Anders Niklasson, Los Alamos National Laboratory, USA

12:35-12:55 Energy Conserving, Linear Scaling, Real Space Ab Initio Molecular Dynamics

Ian Dunn, Columbia University, USA

Friday, March 3

MS317

Application and Algorithm Development using Trilinos - Part II of II

11:20 AM-1:00 PM

Room:218

For Part 1 see MS290

Upon its inception in 2000, the Trilinos project was comprised of a small number of libraries focusing on sparse linear solvers. Since then, the project scope has grown to include many other areas, such as architecture portable computation kernels, fundamental sparse linear algebra, linear and nonlinear solvers, meshing and load balancing, discretization kernels, and uncertainty quantification.The Trilinos user base is distributed among national labs, universities, and companies worldwide. The talks in these minisymposia illustrate the wide breadth of application and library research that is enabled by Trilinos capabilities. Some talks will focus on application areas, e.g., inelastic thermomechanical analysis and reduced order modeling for wind turbine wake modeling, while other talks will discuss development of scientific libraries built using Trilinos capabilities.

Organizer: Christopher Siefert
Sandia National Laboratories, USA

Organizer: Jonathan J. Hu
Sandia National Laboratories, USA

11:20-11:40 Panzer: A Finite Element Assembly Engine within the Trilinos Framework

Jason Gates, Roger Pawlowski, and Eric C. Cyr, Sandia National Laboratories, USA

11:45-12:05 A Novel Algebraic Multigrid Method for Q2-Q1 Discretizations of the Navier-Stokes equations

Andrey Prokopenko, Oak Ridge National Laboratory, USA; Ray S. Tuminaro, Sandia National Laboratories, USA

continued in next column

12:10-12:30 Multiphysics Preconditioning with the MueLu Multigrid Library

Tobias A. Wiesner, Ray S. Tuminaro, Eric C. Cyr, John Shadid, and Jonathan J. Hu, Sandia National Laboratories, USA

12:35-12:55 Porting Spectral/hp Element Framework Nektar++ to Kokkos

Mike Kirby, University of Utah, USA; Chris Cantwell, Martin Vymazal, David Moxey, Jan Eichstaedt, Michael Turner, and Spencer Sherwin, Imperial College, United Kingdom

Friday, March 3

MS318

Progress and Challenges in Extreme Scale Scientific Computing and Data - Part II of II

11:20 AM-1:00 PM

Room:219

For Part 1 see MS291

Extreme scale computing efforts have resulted in numerous advances for multicore, manycore and accelerator based scalable systems. In addition, large-scale simulations must increasingly deal with data management and analysis as a first-class concern. In this minisymposium we present some of the latest work in scalable algorithms and libraries for next generation computing platforms. Furthermore, we discuss efforts to better incorporate data science concerns as a principle component of our scientific workflows.

Organizer: Michael Heroux

Sandia National Laboratories, USA

Organizer: Kengo Nakajima

University of Tokyo, Japan

Organizer: Serge G. Petiton

Université Lille 1 and CNRS, France

11:20-11:40 Convergence Between Big Data and HPC

Serge G. Petiton, Université Lille 1 and CNRS, France; Nahid Emad, University of Versailles, France; Laurent Bobelin, Universite François Rabelais, France

11:45-12:05 Hierarchical Matrices and Low-Rank Methods for Extreme-Scale Solvers

Erik G. Boman, Siva Rajamanickam, and Ray S. Tuminaro, Sandia National Laboratories, USA; Chao Chen and Eric F. Darve, Stanford University, USA

12:10-12:30 Stochastic and Hybrid (Stochastic/Deterministic) Methods for Data and Compute Intensive Problems

Vassil Alexandrov, ICREA, Barcelona Supercomputing Center, Spain

12:35-12:55 Automatic Mapping Operator Construction for a Subspace Correction Method Applied to a Series of Linear Systems

Takeshi Iwashita, Hokkaido University, Japan; Shigeru Kawaguchi, Takeshi Mifune, and Tetsuji Matsuo, Kyoto University, Japan

Friday, March 3

MS319

Stochastic Optimization with Differential Equations: Methods and Applications - Part II of II

11:20 AM-1:00 PM

Room:220

For Part 1 see MS292

Mathematical models involving stochastic (partial) differential equations allow both for an accurate description of physical processes, and to include modeling uncertainties. Stochastic optimization in such models can be used for parameter estimation, noise filtering, uncertainty quantification, and experimental design in the presence of randomness or uncertainties. Due to high complexity of the models and uncertainties, such a process is computationally challenging. This minisymposium brings together mathematicians and engineers to trigger discussions and exchange new ideas in this emerging field. Our talks will range from mathematical analysis through algorithmic design to the results of practical applications.

Organizer: Huanhuan Yang

Florida State University, USA

Organizer: Konstantin Pieper

Florida State University, USA

11:20-11:40 Taylor Approximation for PDE-Constrained Optimal Control Problems Under High-Dimensional Uncertainty: Application to a Turbulence Model

Peng Chen, Omar Ghattas, and Umberto Villa, University of Texas at Austin, USA

11:45-12:05 Simulation Based Optimal Experimental Design: A Measure-Theoretic Perspective

Scott Walsh, University of Colorado, Denver, USA

continued in next column

12:10-12:30 Stochastic Optimization for Turbofan Noise Reduction Using Parallel Reduced-Order Modeling

Huanhuan Yang and Max Gunzburger, Florida State University, USA

12:35-12:55 Estimation of Cardiac Conductivities by a Variational Data Assimilation Approach: Analysis and Validation

Alessandro Barone and Alessandro Veneziani, Emory University, USA; Huanhuan Yang, Florida State University, USA; Flavio H. Fenton, Georgia Institute of Technology, USA; Alessio Gizzi, University Campus Bio-medico of Rome, Italy; Simonetta Filippi, University of Rome La Sapienza, Italy

Friday, March 3

MS320

Finite Element Methods for Weather, Oceans and Climate - Part II of II

11:20 AM-1:00 PM

Room:Crystal AF - 1st Fl

For Part 1 see MS294

Finite elements, including spectral element methods, discontinuous Galerkin methods and compatible finite element methods, provide the flexibility to use non-orthogonal and pseudo-uniform meshes on the sphere, as well as unstructured meshes that can be used in multiresolution and adaptive mesh simulations and to resolve topography and coastlines in ocean models, with the ability to maintain consistency and increase the order of accuracy. Finite element methods now form the basis of a number of dynamical core research groups and ocean modelling groups. The application to oceans, weather and climate brings with it specific issues due to the large range of different time and space scales in the problem. Hence, there are many specific aspects that must be considered, examples include compatibility of discretisations with geophysical balances, timestepping algorithms and linear solvers to deal with the large aspect ratios in ocean and atmosphere shaped domains, conservation of energy, mass, momentum, potential vorticity etc., and integration with physics parameterisations. This is currently a rich and vibrant research area and this minisymposium will consider the breadth of approaches and activities in it.

Organizer: Colin J. Cotter

Imperial College, United Kingdom

Organizer: Andrew McRae

University of Bath, United Kingdom

continued in next column

11:20-11:40 R-Adaptive Mesh Generation for Global Weather Prediction

Andrew McRae, University of Bath, United Kingdom; Colin J. Cotter, Imperial College, United Kingdom; Chris Budd, University of Bath, United Kingdom

11:45-12:05 A Computational Algebra of Hybridization Methods for Ocean and Atmosphere Discretizations

Thomas Gibson, David Ham, and Colin J. Cotter, Imperial College, United Kingdom

12:10-12:30 A Hydrostatic Dynamical Core using Higher-order Structure-Preserving Finite Elements

Chris Eldred, Université Paris 13, France; Thomas Dubos, Ecole Polytechnique, France; Evaggelos Kritsikis, Université Paris 13, France

12:35-12:55 The Acme Spectral Finite Element Non-Hydrostatic Dynamical Core

Mark A. Taylor, Sandia National Laboratories, USA; David M. Hall, University of Colorado Boulder, USA; Paul Ullrich, University of California, Davis, USA; Oksana Guba, Sandia National Laboratories, USA

Friday, March 3

MS321

Uncertainty Quantification in Multi-Scale Systems - Part II of II

11:20 AM-1:00 PM

Room:Crystal CD - 1st Fl

For Part 1 see MS293

Quantifying the uncertainty in multi-scale models has becoming crtical in the modeling of systems characterized by multi-scale behaviors. Uncertainties in different scales exhibit different features, and the propagation and interaction of the uncertainties across scales can have substantial effect on the properties of the system. This minisymposium will explore recent advances in numerical algorithms and applications for uncertainty quantification in multi-scale systems including propagation of uncertainty across different scales or domains (e.g., from continuum to micro-scales), uncertainty of under-resolution simulations (e.g., climate models), and model reduction in multi-scale high-dimensional complex systems (e.g., turbulent flows).

Organizer: Xiu Yang

Pacific Northwest National Laboratory, USA

Organizer: Heng Xiao

Virginia Tech, USA

11:20-11:40 Complex Optimization for Big Computational and Experimental Neutron Datasets

Feng Bao, Oak Ridge National Laboratory, USA

11:45-12:05 Stochastic Dynamics for Cross-Scale Uncertainty Propagation in Molecular Systems

Anh Tran and Yan Wang, Georgia Institute of Technology, USA

12:10-12:30 Conex Splitting Method for Transition State in Phase Field Model

Xiang Zhou and Shuting Gu, City University of Hong Kong, Hong Kong

12:35-12:55 A Multiscale Data-Driven Stochastic Method for Elliptic PDEs with Random Coefficients

Maolin Ci and Thomas Hou, California Institute of Technology, USA; *Zhiwen Zhang*, University of Hong Kong, China

Friday, March 3

MS322

The Modeling of Biological Soft Matter Systems in Fluids - Part II of II

11:20 AM-1:00 PM

Room:301

For Part 1 see MS295

Soft matter encompasses a wide variety of materials, particularly in the area of biology. The dynamics of these soft matter systems in fluids is complex, and advanced modeling techniques are required to gain a fundamental understanding of these systems. The purpose of this minisymposium is to bring together researchers interested in the numerical tools required to model these systems, in addition to the use of these tools to gain a qualitative and quantitative understanding of these complex systems. It is hoped that researchers investigating a wide range of scales will be available, to provide a multiscale view of these important systems.

Organizer: David Salac

State University of New York at Buffalo, USA

11:20-11:40 Stokes Flows for Non-Intact Moving Internal Boundaries

Rolf Ryham and James von Albade, Fordham University, USA

11:45-12:05 Modeling of the Interaction Between a Lipid Bilayer Membrane and a Solid Particle

Yuan-Nan Young, New Jersey Institute of Technology, USA; Howard Stone, Princeton University, USA

12:10-12:30 Dynamics of a Multicomponent Vesicle in Shear Flow

Kai Liu, University of California, Irvine, USA; Gary Marple, University of Michigan, USA; *Shuwang Li,* Illinois Institute of Technology, USA; John Lowengrub, University of California, Irvine, USA; Shravan Veerapaneni, University of Michigan, USA

12:35-12:55 An Implementation of a Variational Immersed Boundary Method for Fluid-Structure Interaction using GRINS and libMesh

Boris Boutkov and Paul Bauman, State University of New York at Buffalo, USA

Friday, March 3

MS323

Computer Aided Clinical Trials + Surgical Planning: CSE meets Clinics - Part II of II

11:20 AM-1:00 PM

Room:302

For Part 1 see MS296

One promising frontiers of CSE is Clinics. After decades of numerical modeling oriented at understanding basic physiopathology, CSE is ready to become part of the clinical routine to support the decision-making process through Clinical Trials and Surgical Planning. This will improve significantly healthcare. It requires a strong interdisciplinary effort to integrate medical processing, scientific computing and statistics. This minisymposium gathers scientists with different background to exchange experiences and draw perspectives of this new frontier of applied mathematics. We will focus on the integration of imaging and computational tools and the reliable prescription of boundary conditions in patient- specific modeling.

Organizer: Alessandro Veneziani

Emory University, USA

Organizer: Ajit P. Yoganathan

Georgia Institute of Technology, USA

11:20-11:40 Patient-Specific Simulations of the Ascending Aorta in Aortopathies

Adelia Sequeira, Instituto Superior Tecnico, Portugal

11:45-12:05 Sickle Cell Anemia and Pediatric Strokes: Computational Fluid Dynamics Analysis in the Middle Cerebral Artery

Manu Platt, Georgia Institute of Technology, USA

12:10-12:30 Software Tools for the Assessment of Cardiovascular Diseases: The Emory Cardiac Toolbox Experience

Marina Piccinelli, Emory University, USA

12:35-12:55 On Optimization Approaches to Boundary Conditions Setting in Computational Hemodynamics

Adrien Lefieux, Alex Viguerie, and Alessandro Veneziani, Emory University, USA

Friday, March 3

MS324

Modeling and Applications with Kinetic and Transport Models - Part II of II

11:20 AM-1:00 PM

Room:303

For Part 1 see MS297

This minisymposum is focused on the role of kinetic and transport theory outside of traditional physics-based modeling applications. Recently developed models in the areas of social and economic sciences, as well as high performance computing will be presented which utilize this theoretical framework.

Organizer: Richard C. Barnard

Oak Ridge National Laboratory, USA

Organizer: Michael Herty

RWTH-Aachen, Germany

11:20-11:40 Mean-Field Optimal Control Hierarchy in Consensus Models

Giacomo Albi, Young-Pil Choi, and Massimo Fornasier, Technische Universität München, Germany; Dante Kalise, Radon Institute for Computational and Applied Mathematics, Austria

11:45-12:05 Econophysical Financial Market Models: A Mean-Field Game Approach

Torsten Trimborn, Martin Frank, and Michael Herty, RWTH-Aachen, Germany

12:10-12:30 Kinetic Models of Conservative Economies with Welfare Thresholds

Kirk Kayser and Dieter Armbruster, Arizona State University, USA; Michael Herty, RWTH-Aachen, Germany; Christian Ringhofer, Arizona State University, USA

12:35-12:55 Meanfield Games and Model Predictive Control

Michael Herty, RWTH-Aachen, Germany

Friday, March 3

MS325

Multi-Scale Modeling and Computation of Active Suspensions - Part II of II

11:20 AM-1:00 PM

Room:304

For Part 1 see MS298

Active suspensions, which can consist micro-swimmers, vesicles, microtubule-motor networks or other types of active particles immersed in liquid, exhibit complex dynamics and patterns. Capturing the interplay between the particles and the surrounding fluid in continuum or agent-based models presents significant challenges as hydrodynamic interactions happen on short and long scales. Added difficulties arise when such suspensions interact with boundaries, and peculiar behavior has been observed in experiments mimicking the suspensions' natural habitats. This minisymposium's goal is to explore recent advances, especially on the computational front, on this emerging and expanding topic.

Organizer: Enkeleida Lushi

Brown University, USA

Organizer: Tong Gao

Michigan State University, USA

11:20-11:40 High-Order Adaptive Time Stepping in Vesicle Suspensions

Bryan Quaife, Florida State University, USA

11:45-12:05 A Fast Platform to Simulating Cellular Assemblies of Semi-Flexible Filaments and Motor Proteins

Ehssan Nazockdast, Abtin Rahimian, Denis Zorin, and Michael J. Shelley, Courant Institute of Mathematical Sciences, New York University, USA

12:10-12:30 Theory of Meiotic Spindle Assembly

Sebastian Fuerthauer, Simons Foundation and New York University, USA; Peter Foster and Daniel Needleman, Harvard University, USA; Michael Shelley, Courant Institute of Mathematical Sciences, New York University, USA

12:35-12:55 The Genesis of "Critters": A Multi-part Story

Blaise Delmotte, Michelle Driscoll, Aleksandar Donev, and Paul Chaikin, Courant Institute of Mathematical Sciences, New York University, USA

Friday, March 3

MS326

Bayesian Optimal Experimental Design for ODE/PDE Models - Part II of II

11:20 AM-12:30 PM

Room:305

For Part 1 see MS299

The challenge of optimal information gathering---for the purpose of inference, prediction, design, or control---pervades fields ranging from geophysics to chemical engineering and beyond. These questions can be formalized through the framework of optimal experimental design. Yet extending classical design methodologies to tackle problems of greater scale and dynamic complexity, and to find optimal sequential designs, requires new algorithms and formulations. This minisymposium will gather a wide variety of approaches focusing on design for large-scale inverse problems and nonlinear models, design in the presence of model error, and the approximation and optimization of information metrics. Relevant techniques include surrogate modeling, model reduction, sparse quadrature, asymptotic approximations, PDE/ODE-constrained optimization, stochastic optimization, transport maps, and approximate dynamic programming. We invite contributions focused on methodology and motivated by engineering and science applications.

Organizer: Xun Huan

Sandia National Laboratories, USA

Organizer: Omar Ghattas

University of Texas at Austin, USA

Organizer: Youssef M. Marzouk

Massachusetts Institute of Technology, USA

11:20-11:40 Optimal Sequential Experimental Design using Adaptive Transport Maps

continued in next column

Xun Huan, Sandia National Laboratories, USA; *Youssef M. Marzouk* and Andrew D. Davis, Massachusetts Institute of Technology, USA

11:45-12:05 Sub-Modularity Based Optimal Experimental Design of Kernelized Mis-Specified Dynamic Model

Gal Shulkind, Massachusetts Institute of Technology, USA; Lior Horesh, IBM Research, USA; Haim Avron, Tel Aviv University, Israel

12:10-12:30 A Measure Space Approach to Optimal Experimental Design

Daniel Walter, Boris Vexler, and Ira Neitzel, Technische Universität München, Germany; Konstantin Pieper, Florida State University, USA

Friday, March 3

MS327

High Performance Computational Scale Bridging for Dual-Phase Steel

11:20 AM-1:00 PM

Room:221

Advanced High Strength Steels (AHSS) provide a good combination of both strength and formability and are therefore applied extensively in the automotive industry, especially in the crash relevant parts of the vehicle. Dual-phase (DP) steel is an example for such AHSS, which is widely employed. The excellent macroscopic behavior of this steel is a result of the inherent micro-heterogeneity and complex interactions between the ferritic phase (weak matrix) and martensitic phase (stiffness increasing inclusions) in the microstructure. For a reliable modeling of DP-steels we have to capture the complex interactions between both phases and therefore the consideration of the micro scale is indispensable for the simulations. In the talks of this minisymposium, different modeling aspects such as crystal plasticity and phase transformations of DP steels are considered at the micro scale. For the computational micro-macro modeling and simulation the well-known FE^2 scale bridging approach is used. It allows for the replacement of the phenomenological material law on the macro scale. In order to bring FE^2 to modern supercomputers, at the micro scale, it is combined with the FETI-DP (finite element tearing and interconnecting) domain decomposition method and with an algebraic multigrid method, resulting in the FE2TI software. Computational results for FE2TI, FETI-DP, and BoomerAMG for more than half a million cores are presented.

Organizer: Axel Klawonn
Universitaet zu Koeln, Germany

continued in next column

Organizer: Oliver Rheinbach
Technische Universität Bergakademie Freiberg, Germany

Organizer: Joerg Schroeder
Universität Duisburg-Essen, Germany

11:20-11:40 FE2TI - Parallel Computational Scale Bridging for Dual-Phase Steels
Oliver Rheinbach, Technische Universität Bergakademie Freiberg, Germany; Axel Klawonn and Martin Lanser, Universitaet zu Koeln, Germany

11:45-12:05 Two-Scale Simulation of Low-Alloyed Trip Steels based on Phase Transformation at the Microscale
Daniel Balzani, Universität Duisburg-Essen, Germany; Ashutosh Gandhi and Stefan Prueger, Technische Universität Dresden, Germany

12:10-12:30 Highly Scalable Implicit Solvers for Elasticity Problems on More Than Half a Million Parallel Tasks
Martin Lanser and Axel Klawonn, Universitaet zu Koeln, Germany; Oliver Rheinbach, Technische Universität Bergakademie Freiberg, Germany

12:35-12:55 Modeling of Polycrystals Using a Fcc/bcc Crystal Visco-Plasticity Theory Applying a Robust Complex-Step Derivative Approximation for the Tangent Moduli
Lisa Scheunemann, Joerg Schroeder, and Daniel Balzani, Universität Duisburg-Essen, Germany; Masato Tanaka, Toyota Central R & D Labs., Inc., Japan

Friday, March 3

CP23

Computational Science - Part II of II

11:20 AM-1:00 PM

Room:224

For Part 1 see CP22

Chair: Kyle E. Niemeyer, Oregon State University, USA

11:20-11:30 Education for Simulation Sciences and HPC at JSC
Johannes Grotendorst, Forschungszentrum Jülich, Germany

11:32-11:42 Modeling Chemical Reactions in Classical Molecular Dynamics Using Data Analytics
Alexander Lohse, Edmond Chow, and Karl Jacob, Georgia Institute of Technology, USA

11:44-11:54 Adaptive Sampling of Carrier Population Data for Multiscale Semiconductor Modeling
Brent Kraczek, US Army Research Laboratory, USA

11:56-12:06 Mathematical Modelling of Love-Type Wave in a Double Layered Piezoelectric Structure
Santan Kumar and Abhishek Singh, Indian School of Mines, India

12:08-12:18 Computation of Derived Variables for the Eddy Current Maxwell's Equations
Christopher Siefert, Sandia National Laboratories, USA; Logan Meredith, University of Rochester, USA; Duncan A. McGregor, Sandia National Laboratories, USA

12:20-12:30 Investigation of Stiffness Detection Metrics for Chemical Kinetics ODEs
Kyle E. Niemeyer, Oregon State University, USA

12:32-12:42 Piecewise Linear Polynomials in Position Dependent Random Maps
Tulsi Upadhyay, University of Southern Mississippi, USA

12:44-12:54 New Algorithms for Solving Multimaterial Diffusion Problems on Meshes Non-Aligned with Material Interfaces
Evgeny Kikinzon and Mikhail Shashkov, Los Alamos National Laboratory, USA; Yuri Kuznetsov, University of Houston, USA

Conference Adjourns

1:00 PM

Notes

Organizer and Speaker Index

SIAM Conference on
Computational Science and Engineering

February 27-March 3, 2017
Hilton Atlanta, Atlanta, Georgia, USA

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CSE17 Budget

Conference Budget
SIAM Conference on Computational Science & Engineering
February 27 - March 3, 2017
Atlanta, GA

Expected Paid Attendance: 1,400

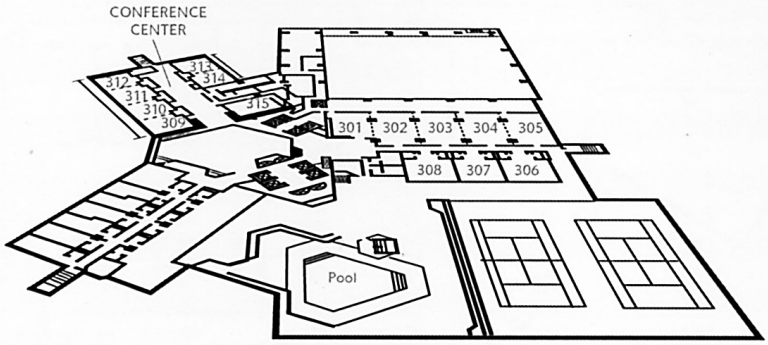
Revenue		
Registration Income		$510,510
	Total	$510,510
Expenses		
Printing		$10,300.00
Organizing Committee		$6,500.00
Invited Speakers		$19,000.00
Food and Beverage		$124,700.00
AV Equipment/ Room Rental and Telecommunication		$118,900.00
Advertising		$7,500.00
Conference Labor (including benefits)		$116,566.00
Professional Services (Recording / Mobile App / Child Care)		$17,900.00
Other (supplies, staff travel, freight, misc.)		$22,500.00
Administrative		$43,391.00
Accounting/Distribution & Shipping		$23,715.00
Information Systems		$43,607.00
Customer Service		$16,339.00
Marketing		$25,218.00
Office Space (Building)		$16,669.00
Other SIAM Services		$17,371.00
	Total	$630,176.00
Net Conference Expense		-$119,666.00
Support Provided by SIAM		$119,666.00
		$0.00

Estimated Support for Travel Awards not included above:

Early Career and Students	83	$68,000

Atlanta Hilton Floor Plan

THIRD FLOOR



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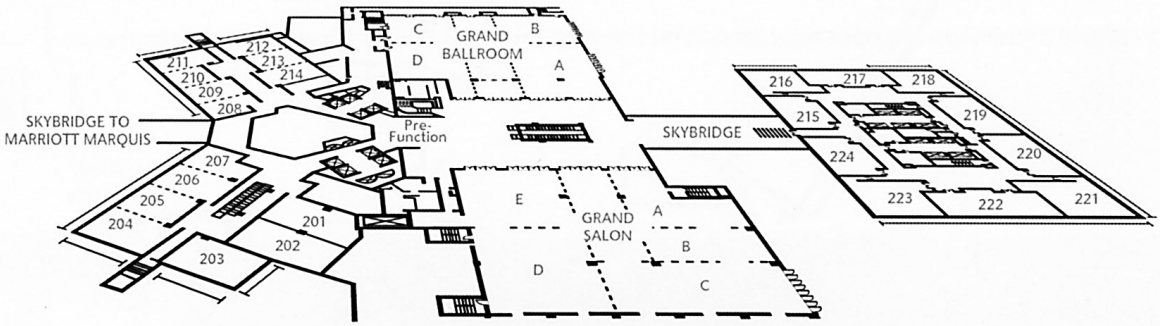

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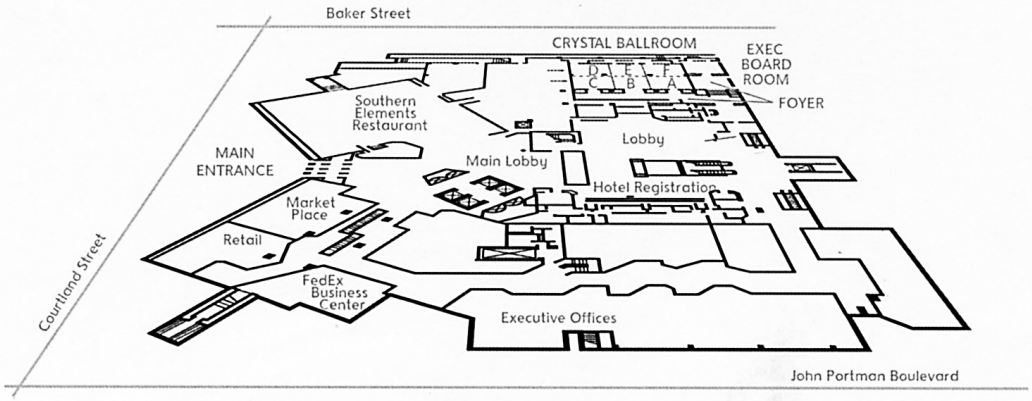

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