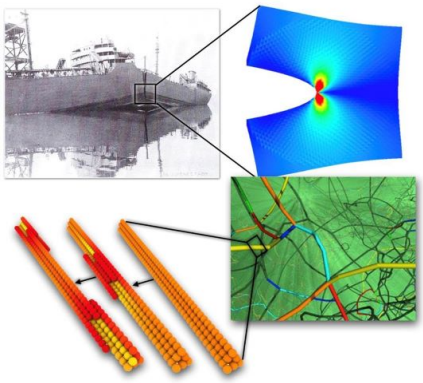
institute for pure & applied mathematics

Workshop II: Scale-Bridging Materials Modeling at Extreme Computational Scales

April 17 - 21, 2023



Scientific Overview

This workshop will focus on new mathematical approaches to multiscale/ multiphysics modeling, with a particular emphasis on the many theoretical and numerical challenges faced at the exascale. The goal is to bring together specialists in a range of massively parallel algorithms and researchers interested in improving the scalability of current techniques.

Topics that will be covered in this workshop include:

- Scalable mathematical formulations for concurrent multi-scale simulations at massive scales.
- Automated derivation of coarse-grained model from massive-scale simulations.
- Uncertainty-quantification-driven parameterization of multiscale models.
- Design of scalable multiscale solvers.
- Implementation of concurrent multiscale models at massive scales.

This workshop will include a poster session; a request for posters will be sent to registered participants in advance of the workshop.

Long Program Schedule

This workshop is part of the long program on "New Mathematics for the Exascale"

- New Mathematics for the Exascale Opening Day: March 13, 2023
- New Mathematics for the Exascale Tutorials: March 14-17, 2023
- Workshop I: Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing: March 27-31, 2023
- **Workshop II: Scale-Bridging Materials Modeling at Extreme Computational Scales: April 17-21, 2023**
- Workshop III: Complex Scientific Workflows at Extreme Computational Scales: May 1-5, 2023
- Workshop IV: Co-design for the Exascale and IPAM Hackathon: May 22-26, 2023
- Culminating Workshop at Lake Arrowhead: June 11-16, 2023

Participation

Additional information about this workshop including links to register and to apply for funding, can be found on the webpage listed below. Encouraging the careers of women and minority mathematicians and scientists is an important component of IPAM's mission, and we welcome their applications.

Organizers

Irene Beyerlein (UCSB), Thomas Hudson (University of Warwick), Thomas Swinburne (CNRS), Anna Vainchtein (University of Pittsburgh)

Invited Speakers

Xiantao Li (Penn State); **Ellad Tadmor** (Minnesota);**Yekaterina Epshteyn** (Univ. Utah); **Maria Emelianenko** (George Mason); **Lev Truskinovsky** (ESPCI); **Elizabeth Holm** (Carnegie Mellon); **Amit Acharya** (Carnegie Mellon); **Florin Bobaru** (Univ. Nebraska); **Ioannis Kevrekidis** (Johns Hopkins); **Genevieve Dusson** (CNRS); **Mark Peletier** (TU Eindhoven); **Upanshu Sharma** (FU Berlin); **Adriana Garroni** (Rome La Sapienza); **Christoph Ortner** (UBC); Gero Freisecke (TU Munich); **Abigail Hunter** (LANL); **Marisol Koslowski** (Purdue); **Liming Xiong** (Iowa State); **James Kermode** (Warwick); **Mihai-Cosmin Marinica** (CEA Saclay); **Alexander Stukowski** (OVITO GmbH); **Laura Ratcliff** (Univ. Bristol); **Arash Mostofi** (Imperial College London); **Gabor Csányi** (Cambridge); and **Celia Reina** (Penn).

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For more information, visit the program web page:

www.ipam.ucla.edu/NMEWS2