

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

Monday April 17, 2023

- 8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome & Opening Remarks: Dean Miguel García-Garibay (Dean of Physical Sciences, UCLA) and Dima Shlyakhtenko (Director, IPAM)*
- 9:00 *SESSION CHAIR: Thomas Hudson (University of Warwick)*
- 9:00–9:50 **Gabor Csányi** (University of Cambridge)
Machine learning potentials: from polynomials to message passing networks
- 10:00–10:15 *Break*
- 10:15–11:05 **Genevieve Dussan** (Université de Franche-Comté (Besançon))
Toward nonlinear reduced basis methods using optimal transport in electronic structure calculations
- 11:15–11:30 *Break*
- 11:30–12:20 **Xiantao Li** (Pennsylvania State University)
A stochastic algorithm for self-consistent field iterations in electron structure calculations.
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Mitchell Luskin** (University of Minnesota, Twin Cities)
Computing at the Moiré Scale
- 3:30–3:50 *Break*
- 3:50–4:40 **Boris Kozinsky** (Harvard University)
Symmetry and uncertainty-aware machine learning models of many-body atomic and electronic interactions
- 4:50–5:15 *Lightning Poster Presentations*
- 5:15–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday April 18, 2023

- 8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *SESSION CHAIR: Anna Vainchtein (University of Pittsburgh)*
- 9:00–9:50 **Lev Truskinovsky** (Laboratoire de Physique et Mécanique des Milieux Hétérogènes)
Mesoscopic tensorial model of crystal plasticity
- 10:00–10:15 *Break*

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- 10:15–11:05 **Shenglin Huang** (University of Pennsylvania)
Data-Driven Model Discovery for Non-equilibrium Processes
- 11:15–11:30 *Break*
- 11:30–12:20 **Florin Bobaru** (University of Nebraska-Lincoln)
Peridynamic models of fracture and damage across scales: enabling large scale computations with fast convolution-based methods
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Yekaterina Epshteyn** (University of Utah)
New perspectives on multiscale modeling and analysis of grain growth in polycrystalline materials
- 3:00–3:15 *Break*
- 3:15–4:05 **Maria Emelianenko** (George Mason University)
Integrating multiscale materials modeling with interpretable automation techniques
- 4:15–4:30 *Break*
- 4:30–5:20 **Robert Lipton** (Louisiana State University)
Fracture as an emergent phenomenon

Wednesday April 19, 2023

- 8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *SESSION CHAIR: Irene Beyerlein (University of California, Santa Barbara (UCSB))*
- 9:00–9:50 **Christoph Ortner** (University of British Columbia)
Atomic Cluster Expansion with and Without Atoms
- 10:00–10:15 *Break*
- 10:15–11:05 **James Kermode** (University of Warwick)
Multiscale and data-driven methods for the simulation of material failure
- 11:15–11:30 *Break*
- 11:30–12:20 **Thomas Swinburne** (Centre National de la Recherche Scientifique (CNRS))
Learning uncertainty-aware models of defect kinetics at scale: discrete and continuous state spaces
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Alexander Stukowski** (OVITO GmbH)
Scaling up Atomistic Simulations: Bridging the Gap to Higher-Scale Representations with Post-Processing Methods
- 3:30–3:50 *Break*

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(Wednesday schedule continued from previous page)

3:50–4:40 **Liming Xiong** (Iowa State University)
Bottom-up Prediction of the Microstructure Evolution in Plastically Deformed Heterogeneous Alloys: Theories, Simulations and Applications

Thursday April 20, 2023

8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*

9:00 *SESSION CHAIR: Thomas Swinburne (Centre National de la Recherche Scientifique (CNRS))*

9:00–9:50 **Thomas Hudson** (University of Warwick)
Atomistic and continuum approaches to nanoscale crystal plasticity

10:00–10:15 *Break*

10:15–11:05 **Abigail Hunter** (Los Alamos National Laboratory)
Mesoscale Investigation of Dislocation-Grain Boundary Interactions in Metals and Alloys

11:15–11:30 *Break*

11:30–12:20 **Hélène Zapolsky** (Université de Rouen (Haute-Normandie))
From mesoscopic to atomistic modelling of phase transformation at large time and length scales

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Jaime Marian** (University of California, Los Angeles (UCLA))
Atomic-level fluctuations in crystal plasticity simulations: Coupling diffusive and mechanical scales"

3:30–3:50 *Break*

3:50–4:40 **Marisol Koslowski** (Purdue University)
Surrogate Hot-spot Models for High-fidelity Simulations of Shock to Detonation Transition

Friday April 21, 2023

8:00–8:55 *Check-In/Breakfast (Hosted by IPAM)*

9:00 *SESSION CHAIR: VIRGINIE EHRLACHER (École Nationale des Ponts-et-Chaussées (ENPC))*

9:00–9:50 **Amit Acharya** (Carnegie Mellon University)
Slow time-scale behavior of fast microscopic dynamics

10:00–10:15 *Break*

10:15–11:05 **Frederic Legoll** (Ecole Nationale Des Ponts et Chaussees (LAMI))
Parareal algorithms for molecular dynamics simulations

11:15–11:30 *Break*

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11:30–12:20 **Sambit Das** (University of Michigan)
*Ab-initio computation of core energetics of pyramidal dislocations in Mg and Mg-Y alloy using DFT-FE:
implications towards ductility enhancement*

12:30–2:30 *Lunch (on your own)*

