

Workshop I: Increasing the Length, Time, and Accuracy of Materials Modeling Using Exascale Computing

Monday March 27, 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: Virginie Ehrlicher (École Nationale des Ponts-et-Chaussées)*
- 9:00–9:50 **Lin Lin** (University of California, Berkeley (UC Berkeley))
Interacting models for twisted bilayer graphene: a quantum chemistry approach
- 10:00–10:15 *Break*
- 10:15–11:05 **Heather Kulik** (Massachusetts Institute of Technology)
Exploring multi-million compound spaces with chemical accuracy using machine learning
- 11:15–11:30 *Break*
- 11:30–12:20 **Aidan Thompson** (Sandia National Laboratories)
The LAMMPS particle simulation package: Bringing together innovative physics models, machine-learning interatomic potentials, and extreme-scale computing resources
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Vikram Gavini (University of Michigan)*
- 2:30–3:20 **Aiichiro Nakano** (University of Southern California (USC))
Quantum Materials Dynamics at the Nexus of Exascale Computing, Artificial Intelligence, and Quantum Computing
- 3:30–3:50 *Break*
- 3:50–4:40 **Anders Niklasson** (Los Alamos National Laboratory)
Quantum-Mechanical Molecular Dynamics for Distributed Computing and AI-hardware
- 4:50–5:15 *Lightning Poster Presentation*
- 5:15–6:30 *Poster Session & Reception (Hosted by IPAM)*



Tuesday March 28, 2023

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Lin Lin (UC Berkeley)*
- 9:00–9:50 **Ramil Mouad** (Seoul National University)
Parallel Replica algorithm for Langevin dynamics and Adaptive Metadynamics
- 10:00–10:15 *Break*
- 10:15–11:05 **Danny Perez** (Los Alamos National Laboratory)
Scalable approaches to long-time atomistic dynamics: a journey to the exascale
- 11:15–11:30 *Break*
- 11:30–12:20 **Manuel Athenes** (Commissariat à l'Énergie Atomique (CEA) - Centre d'Études Nucléaires de Saclay (CENS))
Conditioning schemes for accurately estimating thermodynamic and transport properties of metallic alloys: application to thermo-elasticity and elasto-diffusion.
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Richard Hennig (University of Florida)*
- 2:30–3:20 **Virginie Ehlacher** (École Nationale des Ponts-et-Chaussées)
Sparse approximation of the Lieb functional in DFT with moment constraints (joint work with Luca Nenna)
- 3:30–3:50 *Break*
- 3:50–4:40 **Jaafar El-Awady** (Johns Hopkins University)
Modeling the evolution of representative dislocation structures under high thermo-mechanical conditions during Additive Manufacturing of Alloys

Wednesday March 29, 2023

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Laura Grigori (Sorbonne Université)*
- 9:00–9:50 **David Bowler** (University College London)
Large-scale and linear scaling DFT: why we need it, and how we do it
- 10:00–10:15 *Break*
- 10:15–11:05 **Vikram Gavini** (University of Michigan)
Fast, Accurate and Large-scale Ab-initio Calculations for Materials Modeling
- 11:15–11:30 *Break*

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- 11:30–12:20 **Volker Blum** (Duke University)
Large-scale electronic structure theory in FHI-aims and ELSI
- 12:30–12:40 *Group Photo*
- 12:40–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Eric Cancès (École Nationale des Ponts-et-Chaussées (ENPC))*
- 2:30–3:20 **Reinhold Schneider** (Technische Universität Berlin)
A Multi-Reference Coupled Cluster Method for the Computation of Excited States and Tensor Networks (QC-DMRG)
- 3:30–3:50 *Break*
- 3:50–4:40 **Paul Kent** (Oak Ridge National Laboratory)
Extending the reach and accuracy of Quantum Monte Carlo in materials

Thursday March 30, 2023

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Aidan Thompson (Sandia National Laboratories)*
- 9:00–9:50 **Laura Grigori** (Sorbonne Université)
Recent progress in using randomization for solving linear algebra problems
- 10:00–10:15 *Break*
- 10:15–11:05 **Eric Cancès** (École Nationale des Ponts-et-Chaussées (ENPC))
Error estimators for Density-Functional Theory
- 11:15–11:30 *Break*
- 11:30–12:20 **Steve Fitzgerald** (University of Leeds)
Path integral formulation of stochastic processes: non-equilibrium reaction pathways, hyperdynamics, and enhanced sampling
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair: Graeme Henkelman (University of Texas at Austin)*
- 2:30–3:20 **Daniel Schwen** (Idaho National Laboratory)
Parallel sampling for computing rare event probabilities, inverse Bayesian inference and, uncertainty quantification with MOOSE
- 3:30–3:50 *Break*
- 3:50–4:40 *Panel Discussion*

Friday March 31, 2023

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Danny Perez (Los Alamos National Laboratory)*
- 9:00–9:50 **Vasily V. Bulatov** (Lawrence Livermore National Lab)
A growing challenge: what are we going to do with data generated in exascale simulations?
- 10:00–10:15 *Break*
- 10:15–10:45 **Soumendu Bagchi** (Los Alamos National Laboratory)
Strong Entropic Contributions to Thermally activated Kinetics: A Case-study in Dislocation Nucleation
- 10:45–11:05 **Maciej Buze** (Heriot-Watt University)
Exploring atomistic energy landscapes via bifurcation theory, numerical continuation and deflation techniques
- 11:15–11:30 *Break*
- 11:30–12:20 **Ivan Oleynik** (University of South Florida)
Materials at Extremes: Discovery Science with Exascale Computers and Experiment

