

Workshop III: Complex Scientific Workflows at Extreme Computational Scales

Monday May 1, 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: Ping Yang (Los Alamos National Laboratory)*
- 9:00–9:50 **Jörg Neugebauer** (Max-Planck-Institut für Eisenforschung GmbH)
Enabling next-generation materials science simulations by automated workflows
- 10:00–10:15 *Break*
- 10:15–11:05 **Amedeo Perazzo** (Stanford University)
Workflows for experimental facilities and the digital twin approach
- 11:15–11:30 *Break*
- 11:30–12:20 **Deborah Bard** (Lawrence Berkeley National Laboratory)
The Superfacility Model for Connected Science
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Jan Janssen** (Los Alamos National Laboratory)
pyiron – Rapid-prototyping and Up-scaling Workflows for the Exascale
- 3:30–4:00 *Break*
- 4:00–4:50 **Samuel Blau** (Lawrence Berkeley National Laboratory)
High-Throughput DFT and Monte Carlo for Reaction Networks and Machine Learning
- 5:00–5:15 *Lightning Poster Session*
- 5:15–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday May 2, 2023

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *SESSION CHAIR: Mira Todorova (Max-Planck-Institut für Eisenforschung GmbH)*
- 9:00–9:50 **Claudia Draxl** (Humboldt-Universität)
High-throughput spectroscopy and materials discovery by beyond-DFT workflows and data-analysis frameworks
- 10:00–10:15 *Break*

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- 10:15–11:05 **Alex Aiken** (Stanford University)
Task-Based Programming with Legion
- 11:15–11:30 *Break*
- 11:30–12:20 **Marcus Noack** (Lawrence Berkeley Laboratory)
Advanced Gaussian Process Function Approximation and Uncertainty Quantification for Autonomous Experimentation
- 12:30–2:00 *Lunch (on your own)*
- 2:00–2:50 **Joshua Schrier** (Fordham University)
Creating Complex Scientific Workflows that Reach into the Real World
- 3:00–3:15 *Break*
- 3:15–4:05 **Maxim Ziatdinov** (Oak Ridge National Laboratory)
From Human-Centric to AI-Driven Experimentation Workflows for Materials Characterization
- 4:15–4:30 *Break*
- 4:30–5:20 **Linda Hung** (Toyota Research Institute)
Bridging computation and experiment for energy materials discovery

Wednesday May 3, 2023

- 8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*
- 9:00 *SESSION CHAIR: Joshua Schrier (Fordham University)*
- 9:00–9:50 **Ralf Drautz** (Ruhr-Universität Bochum)
From electrons to the simulation of materials
- 10:00–10:15 *Break*
- 10:15–11:05 **Aurora Clark** (University of Utah)
A holistic, high-dimension perspective on extracting and encoding information in complex chemical systems
- 11:15–11:30 *Break*
- 11:30–12:20 **Nestor Aguirre** (SCM)
Revolutionizing Catalysis Industry through Automated Multiscale Modeling and Active Exploration of Chemical Space
- 12:30–12:45 *Group Photo*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Michele Ceriotti** (École Polytechnique Fédérale de Lausanne (EPFL))
Machine learning for atomic-scale modeling - potentials and beyond
- 3:30–4:00 *Break*

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4:00–4:50 **Dilworth (Dula) Parkinson** (Lawrence Berkeley National Laboratory)
X-ray micro-tomography at the Advanced Light Source and National Energy Research Scientific Computing Center (NERSC) superfacility

Thursday May 4, 2023

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00 *SESSION CHAIR: Amedeo Perazzo (Stanford University)*

9:00–9:50 **Johannes Köster** (Universität Duisburg-Essen)
Transparent, reproducible, and adaptable data analysis with Snakemake

10:00–10:15 *Break*

10:15–11:05 **Johannes Blaschke** (Lawrence Berkeley Laboratory)
ExaFEL: Achieving real-time XFEL data analysis using Exascale Hardware

11:15–11:30 *Break*

11:30–12:20 **Seshu Yamajala** (SLAC National Accelerator Laboratory)
Scaling NumPy applications from 1 CPU to thousands of GPUs

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Juliane Mueller** (National Renewable Energy Laboratory)
Adaptive Computing and multi-fidelity learning

3:30–4:00 *Break*

4:00–4:50 *Discussion*

Friday May 5, 2023

8:00–9:00 *Check-in/Breakfast (hosted by IPAM)*

9:00 *SESSION CHAIR: Jörg Neugebauer (Max-Planck-Institut für Eisenforschung GmbH)*

9:00–9:50 **James Corbett** (Lawrence Livermore National Laboratory)
Flux: a next generation resource manager for HPC and beyond

10:00–10:15 *Break*

10:15–11:05 **Ping Yang** (Los Alamos National Laboratory)
Autonomous Discovery for Separation Sciences

11:15–11:30 *Break*

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11:30–12:20 **Richard Hennig** (University of Florida)
AI-driven workflows for the discovery of novel superconductors (Jason Gibson - Second author)

