New Mathematics for the Exascale: Applications to Materials Science Tutorials

Tuesday March 14, 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)*

9:00–10:15 **Vikram Gavini** (University of Michigan)
DFT 1

10:15–10:45 *Break*

10:45–12:00 **Tim Germann** (Los Alamos National Laboratory)
Molecular Dynamics 1

12:00–12:30 *Core Orientation with IPAM Staff*

12:30–2:00 *Lunch (on your own)*

2:00–3:15 **Johannes Blaschke** (Lawrence Berkeley Laboratory)
Complex Workflows 1

3:15–3:45 *Break*

3:45–5:00 **Erik Draeger** (Lawrence Livermore National Laboratory)
Future Exascale Architectures

Wednesday March 15, 2023

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–10:15 **Vikram Gavini** (University of Michigan)
DFT 2

10:15–10:45 *Break*

10:45–12:00 **Bjoern Enders** (Lawrence Berkeley Laboratory)
Complex Workflows 2

12:00–2:00 *Lunch (on your own)*

2:00–3:15 **Tzanio Kolev** (Lawrence Livermore National Laboratory)
Meso and Macroscale Modeling 1

3:15–3:45 *Break*

3:45–5:00 **Elaine Raybourn** (Sandia National Laboratories)
Sociological Aspects

Thursday March 16, 2023

8:00–9:00	*Check-In/Breakfast (Hosted by IPAM)*
9:00–10:15	**Tzanio Kolev** (Lawrence Livermore National Laboratory) *Meso and Macroscale Modeling 2*
10:15–10:45	*Break*
10:45–12:00	**Evan Weinberg** (Nvidia Corporation) *Virtual Talk: Acceleration techniques*
12:00–2:00	*Lunch (on your own)*
2:00–3:15	**Danny Perez** (Los Alamos National Laboratory) *Molecular Dynamics 2*
3:15–3:45	*Break*
3:45–5:00	**Rahul Gayatri** (Lawrence Berkeley Laboratory) *Intro to NERSC and Performance Analysis Tools 1*

Friday March 17, 2023

8:00–9:00	*Check-In/Breakfast (Hosted by IPAM)*
9:00–10:15	**Thomas Hudson** (University of Warwick) *Virtual Talk: Multiscale Modeling*
10:15–10:45	*Break*
10:45–12:00	**Jack Deslippe** (Lawrence Berkeley Laboratory) *Title not available*

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