

## Workshop III: Cryo-Electron Microscopy and Beyond

### Monday November 14, 2022

- 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: Sriram Subramaniam (UBC)*
- 9:00–9:50 **Steven Ludtke** (Baylor College of Medicine)  
*Contextual Conformational Variability in CryoEM and CryoET using Deep Learning*
- 10:00–10:15 *Break*
- 10:15–11:05 **Carlos Oscar Sorzano** (Centro Nacional de Biotecnología (CSIS))  
*Virtual Talk: Overview of the machine and deep learning needs and trends for Single Particle Analysis by Cryo-Electron Microscopy*
- 11:15–11:30 *Break*
- 11:30–12:20 **Geoffrey Woollard** (University of British Columbia)  
*Using Stochastic variational inference and Computational Optimal Transport for problems in 3D heterogeneity*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Ellen Zhong** (Princeton University)  
*Machine learning for determining protein structure and dynamics from cryo-EM images*
- 3:30–3:50 *Break*
- 3:50–4:40 **Roy Lederman** (Yale University)  
*Approaches for Exploring the Geometry of Molecular Conformations in Cryo-EM*
- 4:50–5:20 *Lightning Poster Presentations*
- 5:20–6:45 *Poster Session & Reception (Hosted by IPAM)*

### Tuesday November 15, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair (AM): Joe Kileel (UT Austin)*
- 9:00–9:50 **Chris Russo** (University of Cambridge)  
*The potential of electron cryomicroscopy in situ: new technology to identify molecules in cells*
- 10:00–10:15 *Break*

*(Tuesday schedule continued on next page)*



*(Tuesday schedule continued from previous page)*

- 10:15–11:05 **Petar Petrov** (University of California, Berkeley (UC Berkeley))  
*Laser phase-contrast transmission electron microscopy and associated computational opportunities*
- 11:15–11:30 *Break*
- 11:30–12:20 **Katerina Naydenova** (University of Cambridge)  
*Molecular structure extrapolation to zero dose with cryoEM*
- 12:30–2:30 *Lunch (on your own)*
- 2:30 *Session Chair (PM): Roy Lederman (Yale)*
- 2:30–3:20 **Serena Yeung** (Stanford University)  
*Virtual Talk: Developing Computer Vision Methods for Segmenting and Analyzing Subcellular Components in Cryo-Electron Tomography*
- 3:30–3:50 *Break*
- 3:50–4:40 **Nikolaus Grigorieff** (University of Massachusetts Medical School)  
*Detecting Distinct 60S Ribosome Maturation Intermediates in Cells by 2D Template Matching*

### Wednesday November 16, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Amit Singer (Princeton)*
- 9:00–9:50 **Mikhail Kudryashev** (Stiftung Max-Delbrück-Centrum für Molekulare Medizin (MDC))  
*Virtual Talk: High throughput, high performance algorithms for high resolution subtomogram averaging*
- 10:00–10:15 *Break*
- 10:15–11:05 **Tamir Bendory** (Tel Aviv University)  
*Recovering small molecular structures using cryo-EM*
- 11:15–11:30 *Break*
- 11:30–12:20 **Joe Kileel** (University of Texas at Austin)  
*Method of moments in cryo-EM*
- 12:30–12:40 *Group Photo*
- 12:40–2:30 *Lunch (on your own)*
- 2:30–3:20 **Frederick Poitevin** (SLAC National Accelerator Laboratory)  
*Amortized Inference of Poses for Ab Initio Reconstruction of 3D Molecular Volumes from Experimental Cryo-EM Images*
- 3:30–3:50 *Break*
- 3:50–4:40 **Tristan Bepler** (New York Structural Biology Center (NYSBC))  
*Detection and segmentation of objects in cryo-electron micrographs using geometric deep learning*

## Thursday November 17, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Wah Chiu (Stanford)*
- 9:00–9:50 **Ayelet Heimowitz** (Ariel University)  
*Virtual Talk: Center of Mass Alignment for Noisy Tomographic Projections*
- 10:00–10:15 *Break*
- 10:15–11:05 **Pilar Cossio** (Flatiron Institute)  
*Structural-ensemble probability refinement using Cryo-EM particles*
- 11:15–11:30 *Break*
- 11:30–12:20 **Abhishek Singharoy** (Arizona State University West)  
*Cryo-EM and beyond: Ensemble refinement, free-energy landscapes and molecular dynamics*
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Yuehaw Khoo** (University of Chicago)  
*New approaches in simulation of transition paths*
- 3:30–3:50 *Break*
- 3:50–4:40 **Sonya Hanson** (Flatiron Institute)  
*Better treatments of pose estimation, temperature, noise, and heterogeneity toward understanding biological temperature sensors via cryo-EM*

## Friday November 18, 2022

- 8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*
- 9:00 *Session Chair: Hong Zhou (UCLA)*
- 9:00–9:50 **Maya Topf** (University of Hamburg)  
*Virtual Talk: Refinement and validation of atomic models in cryo-EM maps using TEMPy2*
- 10:00–10:15 *Break*
- 10:15–11:05 **Carlos Esteve-Yague** (University of Cambridge)  
*Spectral decomposition of atomic structures in heterogeneous cryo-EM*
- 11:15–11:30 *Break*
- 11:30–12:20 **Alberto Bartesaghi** (Duke University)  
*High-throughput cryo-ET: from data acquisition to high-resolution structures*
- 12:30 *Conclusion*

