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*

IPAM strives to provide an inclusive environment free of harassment. IPAM does not tolerate sexual harassment, other forms of harassment, or sexual assault. Please familiarize yourself with our community agreement which includes instructions on reporting incidents by using the QR code to the right.