MDAnalysis

UGM 2025

Tempe, Arizona, USA

Sunday, November 9th

Time Start	Time End	Location	Speaker(s)	Title
9:00 AM	9:15 AM	PSF 186	Oliver Beckstein	Welcome and Opening, General Organization Remarks
9:15 AM	9:45 AM	PSF 186	Hugo MacDermott-Opeskin	MDAnalysis: Present and Future
9:45 AM	10:45 AM	PSF 186	Matthias Heyden	Keynote: Sub-Picosecond Timescale Information in Microsecond Simulations
10:45 AM	11:30 AM	PSF foyer		*Tea / Coffee Break w/ Meet and Greet*
11:30 AM	11:50 AM	PSF 186	Peter Zhang	Ion-Dependent Structural Ensemble and Phase Separation Propensity of Single-Stranded RNA
11:50 AM	12:10 PM	PSF 186	Jennifer A Clark	Hydration Contribution to the Solvation Free Energy of Water-Soluble Polymers
12:10 PM	12:30 PM	PSF 186	Amruthesh Thirumalaiswamy	Studying the Effect of Solvent Crowding on Protein Energy Landscapes
12:30 PM	2:30 PM	PSF foyer		*Lunch and Posters*
2:30 PM	2:50 PM	PSF 186	Matthias Heyden	IMD Streaming Introduction
2:50 PM	3:10 PM	PSF 186	Lawson Woods	IMDv3 Streaming: Theory, Implementation, Technical Details
3:10 PM	3:30 PM	PSF 186	Amruthesh Thirumalaiswamy	IMDv3 in Practice: MD Packages, Performance
3:30 PM	3:45 PM	PSF foyer		*Tea / Coffee Break*
3:45 PM	4:05 PM	PSF 186	Heekun Cho	Streaming Applications Demo (2 Examples)
4:05 PM	5:05 PM	PSF 186	Amruthesh Thirumalaiswamy	Streaming Workshop
5:05 PM	5:25 PM	PSF 186	Jamie Rowe	Integrating MDAnalysis Streaming Analysis with WESTPA
5:25 PM	5:35 PM	PSF foyer		*Tea / Coffee Break*
5:35 PM	5:55 PM	PSF 186	Heekun Cho	Streaming Applications Demo
5:55 PM	6:00 PM	PSF 186	Irfan Alibay	Closing Remarks

Monday, November 10th

Time Start	Time End	Location	Speaker(s)	Title
9:00 AM	9:10 AM	PSH 350	Jennifer A Clark	Opening Remarks
9:10 AM	10:10 AM	PSH 350	Lillian Chong	Keynote: From Protein Structure to Function: Weighted Ensembles Beyond Machine Learning
10:10 AM	10:30 AM	PSH 350	Ricardo Xavier Ramirez	2Danalysis: An Open Source Project to Study Complex Lipid Membranes and Their Interaction with Biopolymers
10:30 AM	10:50 AM	PSH 350	Tyler Reddy	TBA
10:50 AM	11:20 AM	PSH 350		*Tea / Coffee Break*
11:20 AM	11:40 AM	PSH 350	Leah Repa	Membrane-Assisted Transport of Bulky Substrates in a Secondary Active Transporter
11:40 AM	12:00 PM	PSH 350	Prateek Rai	Computer-Aided Discovery and Design of Novel Autotaxin-LPA Signaling Axis Inhibitors to Overcome Cancer Therapeutic Resistance.
12:00 PM	12:20 PM	PSH 350	Alyssa Travitz	Large-Scale Collaborative Assessment of Binding Free Energy Calculations for Drug Discovery using OpenFE
12:20 PM	1:35 PM	PSH 350		*Lunch*
1:35 PM	2:00 PM	PSH 350		Lightning Talks
			Joshua Raphael Uy	Using tICA to Find Causes of Conformational Transitions in Transporters.
			Shubham Kumar Pandey	Unraveling Spectral Shifts in Microbial Rhodopsin through Machine Learning and Molecular Dynamics
			Noah Vasconez	Phosphate Aggregation in Aqueous Solution: Comparison of Non-Polarizable and Polarizable Force Fields
			Matt Kochert	Using a Reservoir-Based Molecular Dynamics Approach to Rapidly Converge New Hamiltonians.
2:00 PM	2:20 PM	PSH 350	Sudheesh Kumar Ethirajan	OPES-Driven Active-Learning Potentials Reveal Node-Assisted Imidazole Diffusion in Flexible SALEM-2 MOF
2:20 PM	2:40 PM	PSH 350	Bryan Gworek	Elucidating the Mechanisms Underlying Phospholipid-Mediated Capsid Formation and Binding between Arc and PI(3)P
2:40 PM	3:00 PM	PSH 350	Brady Johnston	Shining a Ray-Traced Light on Simulations
3:00 PM	3:15 PM	PSH 350		*Tea / Coffee Break*
3:15 PM	3:40 PM	PSH 350		Lightning Talks
			Chris Ausbeck	Directional Coupling and Asymmetry Explain Ligand Specific Allosteric Regulation in LacI
			Danis Yangaliev	Coarse-Grained RNA Model for the Martini 3 Force Field
			Jessica Bodosa	Improving CHARMM36 Force Field for Lipid Interactions with Calcium and Beryllium using Free Energy Perturbation
			Ramón González-Pérez	Exploring the Limits of Ether Oxygen Inclusion in Polymer Membranes for Alkali Ion Separations
3:40 PM	4:00 PM	PSH 350	Augustine Chimezie Onyema	Predicting Interacting Domains in the Nucleosome from Time-Related Kinetic Correlation
4:00 PM	4:20 PM	PSH 350	Chenou Zhang	Conformational Transition of Prestin, the Electro-Mechanical Transducer in Outer Hair Cells of the Inner Ear

Time Start	Time End	Location	Speaker(s)	Title
4:20 PM	4:35 PM	PSH 350		*Tea / Coffee Break*
4:35 PM	4:50 PM	PSH 350	Oliver Beckstein	Master Class: Topology Attributes + DSSP
4:50 PM	5:20 PM	PSH 350	Irfan Alibay	Master Class: Intro to Contributing to MDAnalysis and MDAKits
5:20 PM	5:35 PM	PSH 350	Hugo MacDermott-Opeskin	Master Class: Fast Distance Calculations with Distopia in MDAnalysis
5:35 PM	5:55 PM	PSH 350	Lawson Woods	Master Class: MDAnalysis for ML/Protein Prediction Workflows
5:55 PM	6:00 PM	PSH 350	Irfan Alibay	Closing Remarks

Tuesday, November 11th

Time Start	Time End	Location	Speaker(s)	Title
8:30 AM	8:55 AM	PSF 186	Workshop Presenters	Workshop Installation Clinic
8:55 AM	9:00 AM	PSF 186	Yuxuan Zhuang	Opening Remarks
9:00 AM	11:00 AM	PSF 186	Brady Johnston and Yuxuan Zhuang	Visualization Workshop
11:00 AM	11:20 AM	PSF foyer		*Tea / Coffee Break*
11:20 AM	11:50 AM	PSF 186		Lightning Talks
			Jherome Brylle Woody Santos	A Stratified Nani Approach for Fast and Scalable K-Means Clustering of Large Molecular Dynamics Datasets
			Rekha Joshi	Identification of Specific Interactions between the Membrane Protein Prestin and Lipids
			Pooja Shrestha	TBA
			Jennifer A Clark	ZENO-MDAKit
			Michael A. Sauer	Dynamics-Informed Machine Learning: Physics-Guided Feature Importance Identifies Key Residues for Enzyme Design
11:50 AM	12:00 PM	PSF 186	Irfan Alibay	Intro to the Open Molecular Software Foundation (OMSF)
12:00 PM	1:05 PM	PSF 186	Jeffrey Wagner, Jennifer A Clark	Open Force Field Workshop
1:05 PM	2:20 PM	PSF foyer		*Lunch*
2:20 PM	3:20 PM	PSF 186	Mike Henry, Alyssa Travitz, Irfan Alibay	Open Free Energy Workshop
3:20 PM	3:35 PM	PSF foyer		*Tea / Coffee Break*
3:35 PM	4:35 PM	PSF 186	Hugo MacDermott-Opeskin	OpenADMET Workshop
4:35 PM	4:50 PM	PSF 186	Irfan Alibay	Closing Remarks

Chan Zuckerberg Initiative (CZI)
CZI Grants; 2022-253062 and DAF2021-237663
[DOI: 10.37921/426590wiobus]
From the CZI DAF, an advised fund of Silicon Valley Community Foundation
[DOI: 10.13039/100014989]

U.S. National Science Foundation (NSF)
NSF award 2311372 (Elements: Streaming Molecular Dynamics Simulation Trajectories for Direct Analysis: Applications to Sub-Picosecond Dynamics in Microsecond Simulations)

NumFOCUS
MDAnalysis also thanks NumFOCUS for its continued support as our fiscal sponsor.