



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 | — | <i>Tea / Coffee Break w/ Meet and Greet, group photo, poster set-up</i> |
| 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 | — | <i>Tea / Coffee Break</i> |
| 3:45 PM | 4:05 PM | PSF 186 | Matthias Heyden | Streaming Applications Demo I |
| 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 | — | <i>Tea / Coffee Break</i> |
| 5:35 PM | 5:55 PM | PSF 186 | Matthias Heyden | Streaming Applications Demo II |
| 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 | Modernization of the MDAanalysis Developer Tools |
| 10:50 AM | 11:20 AM | PSH 350 | — | <i>Tea / Coffee Break</i> |
| 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 | — | <i>Lunch</i> |
| 1:35 PM | 2:00 PM | PSH 350 | Joshua Raphael Uy | Lightning Talks 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 | — | <i>Tea / Coffee Break</i> |
| 3:15 PM | 3:40 PM | PSH 350 | Chris Ausbeck | Lightning Talks Directional Coupling and Asymmetry Explain Ligand Specific Allosteric Regulation in LacI |
| | | | Danis Yangaliev | Coarse-Grained RNA Model for the Martini 3 Force Field |
| | | | Jessica Bodoso | 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 | — | <i>Tea / Coffee Break</i> |
| 4:35 PM | 4:50 PM | PSH 350 | Oliver Beckstein | Master Class: Topology Attributes + DSSP |
| 4:50 PM | 5:05 PM | PSH 350 | Hugo MacDermott-Opeskin | Master Class: Fast Distance Calculations with Distopia in MDAnalysis |
| 5:05 PM | 5:35 PM | PSH 350 | Irfan Alibay | Master Class: Intro to Contributing to MDAnalysis and MDAKits |
| 5:35 PM | 5:55 PM | PSH 350 | CoreDevs | Ask me anything: Open Q&A |
| 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 | — | <i>Tea / Coffee Break</i> |
| 11:20 AM | 11:45 AM | PSF 186 | Jherome Brylle Woody Santos | Lightning Talks 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 | Directional Bias Changes in Active Site Region Revealed by Spectral Assignment of Inter-Domain Correlation Mapping in Lysozyme |
| 11:45 AM | 12:00 PM | PSF 186 | Jennifer A Clark Irfan Alibay | ZENO-MDAKit 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 | — | <i>Lunch</i> |
| 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 | — | <i>Tea / Coffee Break</i> |
| 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]

**Chan
Zuckerberg
Initiative** 

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)



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MDAnalysis also thanks NumFOCUS
for its continued support as our fiscal
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