



MDANALYSIS

User Group Meeting

Wednesday, 21 August

King's College London, Bush House, Lecture Theatre 1

Time (BST)	
09:00 - 09:30	Check-In/Registration
09:30 - 09:35	Welcome and Opening Remarks
09:35 - 10:15	MDAnalysis State of the Union
10:15 - 10:45	Coffee Break and Meet and Greet
	Keynote Talk
10:45 - 11:45	<i>Antonia Mey</i> - From a Molecular Movie of a Protein to Quantitative Data
	Applications in Materials Science and Soft Matter
	<i>Josh Dunn</i> - Kinisi: Bayesian Analysis of Mass Transport from Molecular Dynamics Simulations
	<i>Özge Özkılınç</i> - Exploring Lipase Biocatalysis in Sugar-Based Natural Deep Eutectic Solvents for Production of Novel Polymeric Compounds
11:45 - 12:45	<i>Shivani Grover</i> - Choline Based Plastic Crystals as Barocaloric Materials: Insights from Ab Initio Molecular Dynamics
12:45 - 14:15	Lunch
	Toolkit Showcase
	<i>Sarah Fegan</i> - CodeEntropy Software Development
	<i>Raquel López-Ríos de Castro</i> - PySoftK 2.0: Tool for the Analysis of Interfaces, Interactions and Self-Assembly in Soft Matter Simulations
14:15 - 15:15	<i>Hannah Pollak</i> - ClayCode: A Toolkit for Clay Simulation Setup and Analysis
15:15 - 15:45	Coffee Break
	Panel Discussion
	Communities and Resources for Computational Molecular Scientists
15:45 - 16:45	<i>Panelists:</i> Sarah Fegan (CCPBioSim), Shozeb Haider (MGMS), Edina Rosta (TYC), Michelle Sahai (CompChemURG)
	Lightning Talks
	<i>Valerij Talagayev</i> - OpenMMDL: A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis
	<i>Gangarapu Kiran</i> - Molecular Dynamic Simulation of Methotrexate Drug with Silver Nanoparticle in Drug Delivery Across Cell Membrane
	<i>Simon Holtbruegge</i> - Isotropic, Semi-isotropic, and Anisotropic Rotational Diffusion from Molecular Dynamics Trajectories
	<i>Kira Fischer</i> - Calculating Pair Distribution Functions in Anisotropic Geometries
	<i>Asal Azar</i> - Structural Dynamics of a Metalloprotease Enzyme: Insights from Molecular Dynamics Simulations
	<i>Zhiwen Zhong</i> - Unraveling the Molecular Dance: Insights into TREM2/DAP12 Complex Formation in Alzheimer's Disease through Molecular Dynamics Simulations
	<i>Midhun Mohan Anila</i> - Scrutinising the Conformational Ensemble of the Intrinsically Mixed-Folded Protein Galectin-3
16:45 - 17:30	<i>Yu-Yuan (Stuart) Yang</i> - Deep Learning for Binding Site Segmentation in Protein Ensembles
17:30 - 17:35	Day 1 Closing Remarks
17:35 - 21:00	Reception and Poster Session (Bush House, 8th Floor (South))



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Thursday, 22 August

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Time (BST)	
09:00 - 09:25	Check-In/Registration
09:25 - 09:30	Day 2 Opening Remarks
	Keynote Talk
09:30 - 10:30	<i>Francesca Stanzione</i> - Molecular Dynamics for Drug Discovery: Insights into Protein, Ligand, and Protein-Ligand Complexes
10:30 - 11:00	Coffee Break
	Toolkit Showcase
	<i>Ferdoos Hossein Nezhad</i> - MDGraphEmb: A Toolkit for the Encoding of Molecular Dynamics Data Using Graph Embedding
	<i>Namir Oues</i> - MDAutoMut: A Toolkit for the Automated Evaluation of the Impact of Mutations on Protein Dynamics
11:00 - 12:00	<i>Lexin Chen</i> - Molecular Dynamics Analysis with N-ary Clustering Ensembles (MDANCE), A Novel Clustering Package Based on N-ary Similarity
12:00 - 12:45	Everything You Wanted to Know About MDAnalysis, But Didn't Dare Ask!
12:45 - 14:15	Lunch
	Applications in Drug Discovery and Therapeutics
	<i>Hugo MacDermott-Opeskin</i> - Building an Open Source Antiviral Drug Discovery Toolkit
	<i>Evelyn Qiu</i> - Investigating Allosteric Inhibitory Mechanisms of the Soluble Epoxide Hydrolase
	<i>Ivan Man</i> - The Effect of Missense Mutations on the Binding Pocket Dynamics of Skeletal Myosin
14:15 - 15:30	<i>Sana Akhter</i> - Mechanism of Ligand Binding to Target RNA Aptamer
15:30 - 16:00	Coffee Break
	Machine Learning and Multiscale Modeling with MD
	<i>Henrik Stooß</i> - Spatially Resolved Impedance Spectra from Molecular Dynamics Simulations: A Generalised Correlation Analysis Approach
	<i>Michal H. Kolar</i> - Computer Simulations of the Ribosome
	<i>Matteo Degiacomi</i> - Molearn: Streamlining the Design of Generative Models of Biomolecular Dynamics
16:00 - 17:15	<i>Oliver Beckstein</i> - Using MDAnalysis for Machine Learning: Non-parametric Bayesian Kinetic Clustering
17:15 - 17:30	Presentation of Awards and Day 2 Closing Remarks
	(Optional) Social Pub Night (Bermondsey Bierkeller, 2-4 Tooley Street, London, SE1 2SY)
19:00 - 21:00	<i>Pre-registered Attendees (More information to follow via email to those registered for the event)</i>



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Friday, 23 August

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Time (BST)	
09:00 - 09:30	Check-In/Registration
09:30 - 10:15	A Bird's Eye View of Contributing to and Maintaining Open Source Software
10:15 - 10:30	Hackathon Introduction & Project Setup
10:30 - 12:30	Work on Hackathon Projects
12:30 - 14:00	Lunch
14:00 - 16:00	Work on Hackathon Projects
16:00 - 17:00	Project Showcase