



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 - 09:45	Welcome and Opening Remarks
09:45 - 10:45	Keynote Talk <i>Antonia Mey</i> - From a Molecular Movie of a Protein to Quantitative Data
10:45 - 11:15	Coffee Break
11:15 - 12:15	Applications in Materials Science and Soft Matter <i>Andrew McCluskey</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 <i>Shivani Grover</i> - Choline Based Plastic Crystals as Barocaloric Materials: Insights from Ab Initio Molecular Dynamics
12:15 - 12:30	TBD
12:30 - 14:00	Lunch
14:00 - 14:30	MDAnalysis State of the Union
14:30 - 15:30	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 <i>Hannah Pollak</i> - ClayCode: A Toolkit for Clay Simulation Setup and Analysis
15:30 - 16:00	Coffee Break
16:00 - 16:30	TBD
16:30 - 17:15	Lightning Talks <i>Maria Baczynska</i> - Structural Studies into Biofilm Formation by the Legionella Pneumophila Collagen-Like Protein <i>Valerij Talagayev</i> - OpenMMDL: A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis <i>Kiran Gangarapu</i> - Molecular Dynamic Simulation of Methotrexate Drug with Silver Nanoparticle in Drug Delivery Across Cell Membrane <i>Papu Kalita</i> - L1 Metallo- β -Lactamase Antimicrobial Resistance Enzyme: A Computational Reaction Mechanism Study <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
16:30 - 17:15	<i>Asal Azar</i> - TBD
17:15 - 17:30	Day 1 Closing Remarks
17:30 - 21:00	Reception and Poster Session (Bush House, 8th Floor (South))



MDANALYSIS

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Thursday, 22 August

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

Time (BST)	
09:00 - 09:30	Check-In/Registration
09:30 - 09:45	Day 2 Opening Remarks
	Keynote Talk
09:45 - 10:45	<i>Francesca Stanzione</i> - Molecular Dynamics for Drug Discovery: Insights into Protein, Ligand, and Protein-Ligand Complexes
10:45 - 11:15	Coffee Break
	Applications in Drug Discovery and Therapeutics
	<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
	<i>Sana Akhter</i> - Mechanism of Ligand Binding to Target RNA Aptamer
11:15 - 12:30	<i>Hugo MacDermott-Opeskin</i> - Building an Open Source Antiviral Drug Discovery Toolkit
12:30 - 14:00	Lunch
	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
14:00 - 15:00	<i>Lexin Chen</i> - Molecular Dynamics Analysis with N-ary Clustering Ensembles (MDANCE), A Novel Clustering Package Based on N-ary Similarity
15:00 - 15:30	TBD
15:30 - 16:00	Coffee Break
	Machine Learning and Multiscale Modeling with MD
	<i>Henrik Stooß (née Jäger)</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



MD ANALYSIS

User Group Meeting

Friday, 23 August

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

Time (BST)	
09:00 - 09:30	Check-In/Registration
09:30 - 10:00	Hackathon Introduction & Project Setup
10:00 - 12:00	Work on Hackathon Projects
12:00 - 13:30	Lunch Break (<i>NOTE: Lunch will not be provided</i>)
13:30 - 15:30	Work on Hackathon Projects
15:30 - 16:30	Project Showcase