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** *Antonia Mey* - 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** *Andrew McCluskey* - Kinisi: Bayesian Analysis of Mass Transport from Molecular Dynamics Simulations *Özge Özkılınç* - Exploring Lipase Biocatalysis in Sugar-Based Natural Deep Eutectic Solvents for Production of Novel Polymeric Compounds *Shivani Grover* - 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** *Sarah Fegan* - CodeEntropy Software Development *Racquel López-Ríos de Castro* - PySoftK 2.0: Tool for the Analysis of Interfaces, Interactions and Self-Assembly in Soft Matter Simulations *Hannah Pollak* - 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** *Maria Baczynska* - Structural Studies into Biofilm Formation by the Legionella Pneumophila Collagen-Like Protein *Valerij Talagayev* - OpenMMDL: A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis *Kiran Gangarapu* - Molecular Dynamic Simulation of Methotrexate Drug with Silver Nanoparticle in Drug Delivery Across Cell Membrane *Papu Kalita* - L1 Metallo- β -Lactamase Antimicrobial Resistance Enzyme: A Computational Reaction Mechanism Study *Simon Holtbruegge* - Isotropic, Semi-isotropic, and Anisotropic Rotational Diffusion from Molecular Dynamics Trajectories *Kira Fischer* - Calculating Pair Distribution Functions in Anisotropic Geometries *Asal Azar* - TBD
17:15 - 17:30	Day 1 Closing Remarks
17:30 - 21:00	**Reception and Poster Session (Bush House, 8th Floor (South))**

MDANALYSIS User Group Meeting

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
09:45 - 10:45	**Keynote Talk** *Francesca Stanzione* - Molecular Dynamics for Drug Discovery: Insights into Protein, Ligand, and Protein-Ligand Complexes
10:45 - 11:15	Coffee Break
11:15 - 12:30	**Applications in Drug Discovery and Therapeutics** *Evelyn Qiu - Investigating Allosteric Inhibitory Mechanisms of the Soluble Epoxide Hydrolase* *Ivan Man - The Effect of Missense Mutations on the Binding Pocket Dynamics of Skeletal Mysoin* *Sana Akhter* - Mechanism of Ligand Binding to Target RNA Aptamer *Hugo MacDermott-Opeskin* - Building an Open Source Antiviral Drug Discovery Toolkit
12:30 - 14:00	Lunch
14:00 - 15:00	**Toolkit Showcase** *Ferdoos Hossein Nezhad* - MDGraphEmb: A Toolkit for the Encoding of Molecular Dynamics Data Using Graph Embedding *Namir Oues* - MDAutoMut: A Toolkit for the Automated Evaluation of the Impact of Mutations on Protein Dynamics *Lexin Chen* - 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
16:00 - 17:15	**Machine Learning and Multiscale Modeling with MD** *Henrik Stooß (née Jäger)* - Spatially Resolved Impedance Spectra from Molecular Dynamics Simulations: A Generalised Correlation Analysis Approach *Michal H. Kolar* - Computer Simulations of the Ribosome *Matteo Degiacomi* - Molearn: Streamlining the Design of Generative Models of Biomolecular Dynamics *Oliver Beckstein* - Using MDAnalysis for Machine Learning: Non-parametric Bayesian Kinetic Clustering
17:15 - 17:30	Presentation of Awards and Day 2 Closing Remarks

MDANALYSIS 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 (*NOTE: Lunch will not be provided*)
13:30 - 15:30	Work on Hackathon Projects
15:30 - 16:30	Project Showcase