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
10:45 - 11:45	**Keynote Talk** *Antonia Mey* - From a Molecular Movie of a Protein to Quantitative Data
11:45 - 12:45	**Applications in Materials Science and Soft Matter** ***Josh Dunn*** - 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
12:45 - 14:15	Lunch
14:15 - 15:15	**Toolkit Showcase** *Sarah Fegan* - CodeEntropy Software Development *Raquel 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
15:15 - 15:45	Coffee Break
15:45 - 16:45	**Panel Discussion** Communities and Resources for Computational Molecular Scientists *Panelists*: Sarah Fegan (CCPBioSim), Shozeb Haider (MGMS), Edina Rosta (TYC), Michelle Sahai (CompChemURG)
16:45 - 17:30	**Lightning Talks** *Valerij Talagayev* - OpenMMDL: A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis *Gangarapu Kiran* - Molecular Dynamic Simulation of Methotrexate Drug with Silver Nanoparticle in Drug Delivery Across Cell Membrane *Simon Holtbruegge* - Isotropic, Semi-isotropic, and Anisotropic Rotational Diffusion from Molecular Dynamics Trajectories *Kira Fischer* - Calculating Pair Distribution Functions in Anisotropic Geometries *Asal Azar* - Structural Dynamics of a Metalloprotease Enzyme: Insights from Molecular Dynamics Simulations *Zhiwen Zhong* - Unraveling the Molecular Dance: Insights into TREM2/DAP12 Complex Formation in Alzheimer's Disease through Molecular Dynamics Simulations *Midhun Mohan Anila* - Scrutinising the Conformational Ensemble of the Intrinsically Mixed-Folded Protein Galectin-3 *Yu-Yuan (Stuart) Yang* - 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))**

MDANALYSIS User Group Meeting

Thursday, 22 August	
King's College London, Bush House, Lecture Theatre 1	
Time (BST)	
09:00 - 09:25	Check-In/Registration
09:25 - 09:30	Day 2 Opening Remarks
09:30 - 10:30	**Keynote Talk** *Francesca Stanzione* - Molecular Dynamics for Drug Discovery: Insights into Protein, Ligand, and Protein-Ligand Complexes
10:30 - 11:00	Coffee Break
11:00 - 12:00	**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
12:00 - 12:45	Everything You Wanted to Know About MDAnalysis, But Didn't Dare Ask!
12:45 - 14:15	Lunch
14:15 - 15:30	**Applications in Drug Discovery and Therapeutics** *Hugo MacDermott-Opeskin* - Building an Open Source Antiviral Drug Discovery Toolkit *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
15:30 - 16:00	Coffee Break
16:00 - 17:15	**Machine Learning and Multiscale Modeling with MD** *Henrik Stooß* - 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
19:00 - 21:00	**(Optional) Social Dinner** *Pre-registered Attendees (More information to follow via email to those registered for the UGM)*

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 - 10:15	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 Break (*NOTE: Lunch will not be provided*)
14:00 - 16:00	Work on Hackathon Projects
16:00 - 17:00	Project Showcase