MDANALYSIS User Group Meeting

Wednesday, 21 August	
King's College London, Bush House, Auditorium	
Time (BST)	
09:00 - 09:30	Check-In/Registration
09:30 - 09:35	Welcome and Opening Remarks (*Oliver Beckstein)*
09:35 - 10:15	MDAnalysis State of the Union *(Richard Gowers)*
10:15 - 10:45	Coffee Break and Meet and Greet (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
10:45 - 11:45	**Keynote Talk** (*Chair: Micaela Matta)* *Antonia Mey* - From a Molecular Movie of a Protein to Quantitative Data
11:45 - 12:45	**Applications in Materials Science and Soft Matter** *(Chair: Micaela Matta)* *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 (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
14:15 - 15:15	**Toolkit Showcase** *(Chair: Fiona Naughton)* *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 (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
15:45 - 16:45	**Panel Discussion** *(Moderator: Hugo MacDermott-Opeskin)* 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** *(Chair: Yuxuan Zhuang)* *Valerij Talagayev* - OpenMMDL: A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes Setup, Simulation and Analysis *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 *(Micaela Matta)*
17:35 - 21:00	**Reception and Poster Session** (Bush House, 8th Floor (South), https://www.kcl.ac.uk/kingsvenues/rooms/bh-8fs)

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09:00 - 09:25	Check-In/Registration
09:25 - 09:30	Day 2 Opening Remarks *(Fiona Naughton)*
09:30 - 10:30	**Keynote Talk** *(Chair: Fiona Naughton)* ***Francesca Stanzione* - Molecular Dynamics for Drug Discovery: Insights into Protein, Ligand, and Protein-Ligand Complexes**
10:30 - 11:00	Coffee Break (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
11:00 - 12:00	**Toolkit Showcase** *(Chair: Hugo MacDermott-Opeskin)* *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! *(Chair: Richard Gowers)*
12:45 - 14:15	Lunch (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
14:15 - 15:30	**Applications in Drug Discovery and Therapeutics** *(Chair: Richard Gowers)* *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 (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
16:00 - 17:15	**Machine Learning and Multiscale Modeling with MD** *(Chair: Yuxuan Zhuang)* *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 *(Oliver Beckstein)*
19:00 - 21:00	**(Optional) Social Pub Night** (Bermondsey Bierkeller, 2-4 Tooley Street, London, SE1 2SY, https://www.bermondseybierkeller.co.uk/) *Pre-registered Attendees*

MDANALYSIS User Group Meeting

Friday, 23 August	
King's College London, Bush House, Auditorium	
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 *(Oliver Beckstein; Fiona Naughton)*
10:15 - 10:30	Hackathon Introduction & Project Setup *(Yuxuan Zhaung, Hugo MacDermott-Opeskin)*
10:30 - 12:30	Work on Hackathon Projects
12:30 - 14:00	Lunch (Bush House Arcade, https://www.kcl.ac.uk/kingsvenues/rooms/bh-arcade)
14:00 - 16:00	Work on Hackathon Projects
16:00 - 17:00	Project Showcase (*Chair: Yuxuan Zhuang, Hugo MacDemott-Opeskin)*

We would like to give a special thanks to our partners and sponsors for this workshop, the Thomas Young Centre (TYC), Chan Zuckerberg Initiative (CZI), and Molecular Graphics and Modelling Society (MGMS). MDAnalysis also thanks NumFOCUS for its continued support as our fiscal sponsor.