MDANALYSIS User Group Meeting

Wednesday, 27 September 2023	
Faculty of Sciences of the University of Lisbon (ULisboa) Auditorium, Building C1	
Time (WEST)	
12:00 - 12:30	Check-In/Registration
12:30 - 12:45	Welcome & Opening Notes
12:45 - 13:30	MDAnalysis State of the Union
13:30 - 14:15	**Applications in Materials Science** *Nisha Middleton* - Atomistic Simulations of Polymers for Sustainable Food Packaging Design *Maria Castellanos* - Integrating Molecular Dynamics and Excited-State Quantum Mechanics for High-Throughput Screening of Molecules in Macromolecular Scaffolding
14:15 - 14:45	Coffee Break (Building C6)
14:45 - 15:45	**Panel Discussion** Careers in MD and Open Source Software
15:45 - 16:30	**Deep Learning and Multiscale Modeling with MD** *Andres Arango* - Topological Learning Approach to Estimating Lipid Temperatures *Oliver Beckstein* - From Transporter Structure to Function via Multiscale Modelling
16:30 - 16:45	Quick Break
16:45 - 17:45	**Keynote Talk** *Giovanni Pavan* - New Paradigms in the Analysis of Innately Dynamic Complex Molecular Systems
17:45 - 18:00	Day 1 Closing Remarks
19:30 - 21:00	Conference Dinner (Rice ME, https://www.riceme.pt/)

MDANALYSIS User Group Meeting

Thursday, 28 September 2023	
Faculty of Sciences of the University of Lisbon (ULisboa) Auditorium, Building C1	
Time (WEST)	
9:00 - 9:30	Check-In/Registration
9:30 - 10:15	**Applications in Drug Discovery** *Hannah Baumann* - Breaking Free from Ligand Similarity Restrictions in Binding Free Energy Calculations *Fiona Naughton* - Investigating Conformational Changes in Membrane Transport Proteins with Molecular Simulation
10:15 - 10:45	**Lightning Talks 1** *Pegerto Fernández* - Graph Learning Workflow for Allosteric Pocket Detection *Melissa Mitchell* - Developing Multiscale Models to Study Molecular Transport into Tissues *Hocine El Khaoudi Enyoury* - G Protein-Coupled Receptor Kinase 2 (GRK2) in Complex with the Neurotensin Receptor 1: A Dynamic Overview *Francesca Stanzione* - Molecular Dynamics at Sosei Heptares
10:45 - 11:15	Coffee Break (Building C6)
11:15 - 12:00	**Toolkit Showcase** *Ian Kenney* - MDAKits: A Framework for FAIR-Compliant Molecular Simulation Analysis *Henrik Jäger* - MAICoS: A Toolkit for the Molecular Analysis of Interfacial and Confined Systems
12:00 - 12:15	Quick Break
12:15 - 13:00	**Toolkit Showcase** *Namir Oues* - MDSubSampler: A Toolkit to Extend MDAnalysis Capability to a Posteriori Sampling of Important Protein Conformations and Data Preparation for Machine Learning *Egor Marin* - Parallelization of MDAnalysis
13:00 - 14:00	Lunch (Building C6)
14:00 - 15:00	**Keynote Talk** *Cédric Bouysset* - Encoding Interactions as Fingerprints in MD Simulations
15:00 - 15:30	**Lightning Talks 2** *Dimitris Stamatis* - Identifying Interaction Patterns and Hotspots in Aggregates of Self-Assembling Biomaterials *Hannah Pollak* - ClayCode: A Tool for Automating the Setup of Atomistic Clay Models for Molecular Dynamics Simulations with GROMACS *Daniel dos Santos* - Using MDAnalysis to Squeeze Simulation Trajectories of ABC Efflux Transporters to get Scientific Insights
15:30 - 16:00	Coffee Break (Building C6)
16:00 - 17:00	**Open Discussion** MDAnalysis and the Future: Defining the Path Forward Beyond 3.0
17:00 - 17:30	Presentation of Awards and Wrap Up

MDANALYSIS User Group Meeting

Friday, 29 September 2023	
SANA Metropolitan Hotel Madrid Room	
Time (WEST)	
9:30 - 10:00	Check-In/Registration
10:00 - 10:30	Hackathon Introduction & Project Setup
10:30 - 12:00	Work on Hackathon Projects
12:00 - 13:00	Lunch (Foyer)
13:00 - 14:30	Work on Hackathon Projects
14:30 - 15:00	Project Showcase