



# 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	<b>Applications in Materials Science</b> <i>Nisha Middleton</i> - Atomistic Simulations of Polymers for Sustainable Food Packaging Design <i>Maria Castellanos</i> - 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	<b>Panel Discussion</b> Careers in MD and Open Source Software
15:45 - 16:30	<b>Deep Learning and Multiscale Modeling with MD</b> <i>Andres Arango</i> - Topological Learning Approach to Estimating Lipid Temperatures <i>Oliver Beckstein</i> - From Transporter Structure to Function via Multiscale Modelling
16:30 - 16:45	Quick Break
16:45 - 17:45	<b>Keynote Talk</b> <i>Giovanni Pavan</i> - 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, <a href="https://www.riceme.pt/">https://www.riceme.pt/</a> )



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Thursday, 28 September 2023

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



# MD ANALYSIS

## 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