Biomolecular Simulations

26th - 28th November 2024

Coimbra, Portugal

Bioexcel Meeting Program

Tuesday 26th November

13:30 - 14:00 Registration

Afternoon session: *Introduction to GROMACS: from basis to advance features* - Alessandra Villa KTH, Stockholm, Sweden

14:00 - 15:00 Theoretical part

Coffee break

15:15 - 16:45 Tutorial - Alessandra Villa & Andrey Alekseenko, KTH, Stockholm, Sweden

Coffee break

GROMACS performance & competition (only for physical attendees)

17:00 - 17:45 Theoretical part: *GROMACS performance*

Coffee break

18:00 - 19:00 *GROMACS performance tutorial & competition*

Wednesday 27th November

Morning session: *HADDOCK: Integrative modeling of biomolecular complexes* - Alexandre Bonvin, Utrecht University, Netherlands

09:45-10:45 Theoretical part

Coffee break

11:00-12:30 Tutorial - Alexandre Bonvin & Victor Rey, Utrecht University, Netherlands

Lunch break

Afternoon session: *Alchemical free energy calculations with PMX/GROMACS* - Bert de Groot, Max Planc Institute, Germany

14:00 - 15:00 Theoretical part: *Introduction into alchemical free energy calculations*

Coffee break

15:15 - 16:45 Tutorial: *Alchemical free energy calculations with PMX/GROMACS* - Bert de Groot & Sudarshan Behera, Max Planc Institute, Germany

17:00 - 18:00 Tour of the University of Coimbra

20:00 Social dinner at O'Papa restaurant

Thursday 28th November

Morning session: *AlphaFold 2.0* - Paulyna Magaña, EMBL-EBI, UK

09:00-10:00 Theoretical part: *AlphaFold2 and its impact on biological research*

Coffee break

10:15-11:45 Tutorial

Coffee break

12:00-12:30 *User-friendly cloud HPC with Python and the Inductiva API* - Hugo Penedones, Inductiva.AI, Portugal

Lunch break

Afternoon session: *BioExcel Building Blocks (BioBB), a software library for interoperable biomolecular simulation workflows* - Pau Andrio & Pieter Zanders, IRB Barcelona, Spain

14:30 - 15:30 Theoretical part: *BioExcel Building Blocks (BioBB), a software library for interoperable biomolecular simulation workflows*

Coffee break

15:45 - 17:15 Tutorial: *BioBB interactive Jupyter Notebooks for FAIR and reproducible biomolecular simulation workflows. Automatic Ligand Parameterization and Protein Conformational Transitions Calculations as examples*