

High Performance Molecular Dynamics: Theory and Applications

This lecture will introduce the basics of molecular dynamics simulations techniques. Both theoretical background and practical aspects of simulation techniques will be addressed. Tutorials will provide test cases of MD simulations using basic examples of running MD simulations on High Performance Calculations (HPC) clusters with state-of-art hardware. By understanding better the HPC infrastructures and the algorithms used to exploit them, the aim is to give the students the tools to run simulations in the most efficient way possible on current and future supercomputers. During the course students will be guided on how to prepare and run simulations on Cineca's HPC systems with the GROMACS application, one of the most common and efficient molecular dynamics applications available. This lecture will cover the following:

- Introduction to classic molecular dynamics
- parallelization schemes in MD simulations
- Optimization of MD performance on HPC clusters
- Hands-on and tutorials

Multi-scale molecular dynamics of biomolecules

Coarse-grained molecular dynamics provides a means for simulating the assembly and the interactions of membrane protein/lipid complexes at a reduced level of representation, allowing longer and larger simulations. Multi-scale simulation techniques are an applications of molecular dynamics algorithms to different level of complexity in biology and chemistry, providing structural and chemical information at different time and spatial scale of biological processes to investigate the nature of biological processes at their typical timescale. In particular, this lecture introduce the main computational techniques related to multi-scale simulations by providing the student with computational tools to run and analyse multi-scale simulation trajectories. This lecture will cover the following subjects:

- Introduction to coarse-grained simulations
- Mesoscale dynamics techniques
- MARTINI forcefield and applications to biomolecules
- Hands-on and tutorials