High Performance Molecular Modelling

11th-13th May 2026, Casalecchio di Reno, CINECA

Teachers: Andrew Emerson, Alessandro Grottesi, Giorgia Frumenzio, Balasubramanian Chandramouli, Lara Querciagrossa

Agenda

11th May – HPC and MD theory

9.30 – 10.00	Registration
10.00 – 11.00	Introduction to HPC architectures and parallelism (A. Emerson)
11.00 – 11.30	Coffee break
11.30 – 12.30	Introduction to Classic Molecular Dynamics (G: Frumenzio)
12.30 – 14.00	Lunch break
14.00 – 15.00	Parallel Molecular Dynamics (A. Emerson)
15.00 – 15.30	Coffee break
15.30 – 17.30	Hands-On: Introduction to CINECA HPC (A. Grottesi)

12th May – Running simulations and AI for MD

9.30 – 10.15	Presentation: MD on GPU Architectures (A. Grottesi)
10.15 – 11.00	Hands-on: MD with OpenMM (A. Grottesi)
11.00 – 11.30	Coffee break
11.30 – 12.30	Hands on: High Throughput MD
12.30 – 14.00	Lunch break
14.00 – 15.30	Use of AI in Molecular Dynamics (L. Querciagrossa)
15.30 - 16.00	Coffee break
16.00 – 17.30	Running MD with OpenMM and AI-generated potentials

Commented [AG1]: Hands on: Strong scaling tutorial with a large (100k atoms) system

13th May – Analysis and Project applications

9.30 – 10.30	Invited speaker: Laura Rigobello, PhD student Univ. Bologna “Parametrization with the Grappa Machine Learning ForceField”
10.30 – 11.00	Coffee break
11.00 – 12.30	Analysis of MD simulations (B. Chandramouli)
12.30 – 14.00	Lunch Break
14.00 – 15.00	How to apply for EuroHPC computer resources (A. Emerson)
15.00 – 17.00	Free Exercises