

High Performance Molecular Modelling

12th-14th May 2025, CINECA

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<https://euroccitaly.it/en/news/hpc-molecular-modelling-a-new-eurocc-course-between-italy-and-lithuania/>

Agenda

12th May – theory + usage di HPC

9.00 – 9.30	Registration
9.30 – 10.15	Introduction to HPC architectures and parallelism (A. Emerson)
10.15 – 10.30	Coffee break
10.30 – 11.30	Introduction to Classic Molecular Dynamics (L. Querciagrossa)
12.30 – 14.00	Lunch break
13.00 – 14.00	Parallel Molecular Dynamics (A. Emerson)
14.00 – 14.30	Coffee break
14.30 – 16.30	Hands-On: Introduction to CINECA HPC (A. Grottesi)

13th May – Running simulations

9.00 – 9.45	Presentation: MD on GPU Architectures (A. Grottesi), incl Amber
9.45 – 10.30	Hands-on: MD with large systems (A. Grottesi)
10.30 – 10.45	Coffee break
10.45 – 11.45	Invited speaker: title: TBA
11.45 – 13.15	Lunch break Running Metadynamics Simulations
13.15 – 15.15	Hands on: preparation for long simulations
15.15 – 16.15	Coffee break
16.15 – 16.45	Introduction to Trajectory Analysis (G. Frumenzio)

14th May - Analysis

9.00 – 10.30	Python Analysis of MD trajectories (B. Chandramouli).
10.30 – 11.00	Coffee break
11.00 – 12.30	Hands-on. Analysis of MD simulations (G. Frumenzio)
12.30 – 14.00	Lunch Break
14.00 – 14.45	How to apply for EuroHPC resources (A. Emerson)
14.45 – 17.00	Questions and Answers