

High Performance Molecular Dynamics

10th -12th May 2023, CINECA, Casalecchio di Reno

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

Agenda

Day 1

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 (L. Querciagrossa)
12.30 – 14.00	Lunch break
14.00 – 15.00	Parallel Molecular Dynamics (G. Frumenzio)
15.00 – 15.30	Coffee break
15.30 – 17.30	Hands-On: Introduction to CINECA HPC (A. Grottesi and N. Besker)

Day 2

9.30 – 10.15	MD on GPU Architectures (A. Grottesi)
10.15 – 11.00	Hands-on: MD practice with scripts and benchmarks (A. Grottesi & N. Besker)
11.00 – 11.30	Coffee break
11.30 – 12.30	Hands-on (continued)
12.30 – 14.00	Lunch break
14.00 – 15.30	Hands-on: more practice and job optimization (A. Grottesi & N. Besker)
15.30 – 16.00	Coffee break
16.00 – 17.30	Hands-on: job optimization for a long trajectory, comparison M100 and Leonardo.

Day 3

9.30 – 11.00	Analysis of MD trajectories (G. Frumenzio and B. Chandramouli).
11.00 – 11.30	Coffee break
11.30 – 13.00	Hands-on. Analysis of MD simulations with Python Notebooks on Galileo100(B. Chandramouli)
13.00 – 14.30	Lunch Break
14.30 – 15.30	Invited Lecturer: F. Musiani, Uni. Bologna (title TBD)
15.30 - 16.00	How to apply for HPC resources (A. Emerson)
15.00 – 17.00	FREE