High Performance Molecular Dynamics

March 26th - 27th - 28th 2018

CINECA – Roma, Sala Corsi, via dei Tizii 6B

Teachers: Andrew Emerson, Giovanni Chillemi, Neva Besker, Alessandro Grottesi

Agenda

March 26th

9.30 – 10.15	Registration
10.15 – 11.00	Introduction to HPC architectures I (A. Emerson)
11.00 – 11.30	Coffee break
11.30 – 12.30	Introduction to Classic Molecular Dynamics (G.Chillemi)
12.30 – 14.00	Lunch break
14.00 – 15.10	MD: Atom, Force and Domain Decomposition (A. Emerson)
15.10 – 15.30	Coffe break
15.30 – 17.30	Tutorial 1: UNIX Environment@ CINECA: PBS and SLURM scheduler (A. Grottesi & N. Besker)

March 27th

9.30 – 10.15	MD on HPC Architectures: GPU, Intel Xeon Phi, KNL, Skylake (A. Grottesi)
10.15 – 11.00	Tutorial 2: MD @ CINECA, scripts and benchmarks (A. Grottesi & N. Besker)
11.00 – 11.30	Coffee break
11.30 – 12.30	Tutorial 3: scalability test for biological systems (A. Grottesi & N. Besker)
12.30 – 14.00	Lunch break
14.00 – 15.00	Tutorial 4: Analysis of MD trajectories (N. Besker)
15.00 – 15.30	Coffee break

15.30 – 17.30	Tutorial 5: Running and analysis using GROMACS and NAMD (A. Grottesi & N. Besker)

March 28th

10.00 – 10.30	Advanced Molecular Dynamics techniques and benchmarks (A. Emerson & A. Grottesi
10.30 – 13.00	Tutorial 6: Essential Dynamics of Proteins (N. Besker)
12.30 – 14.00	Lunch Break
14.00 – 14.30	Access to CINECA HPC resources @ CINECA (A. Emerson)
14.30 -	Free