

# High Performance Molecular Dynamics

14<sup>th</sup> -16<sup>th</sup> October 2019

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

Teachers: Andrew Emerson, Neva Besker,  
Alessandro Grottesi

## Agenda

### Monday 14<sup>th</sup> October

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 (A. Grottesi)
12.30 – 14.00	Lunch break
14.00 – 15.10	MD: Atom, Force and Domain Decomposition (A. Emerson)
15.10 – 15.30	Coffee break
15.30 – 17.30	Tutorial 1: UNIX Environment@ CINECA: PBS and SLURM scheduler (A. Grottesi)

### Tuesday 15<sup>th</sup> October

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	External speaker (TBD).
12.30 – 14.00	Lunch break
14.00 – 15.30	Tutorial 3: scalability test for biological systems (A. Grottesi & N. Besker)
15.30 – 16.00	Coffee break
16.00 – 17.30	Tutorial 4: Running and analysis of MD trajectories (N. Besker)

## Wednesday 16<sup>th</sup> October

9.30 – 11.00	Advanced Molecular Dynamics techniques and benchmarks (A. Emerson & A. Grottesi)
11.00 – 11.30	Coffee break
11.30 – 13.00	Tutorial 5: Essential Dynamics of Proteins (N. Besker)
13.00 – 14.00	Lunch Break
14.00 – 14.30	Access to CINECA HPC resources @ CINECA (N. Besker)
14.30 – 17.30	Free exercises and tutorials.