

High Performance Molecular Dynamics*

28-30 September 2016

Cineca – Bologna (KION), Via Magnanelli 2, 40033 Casalecchio di Reno.

Instructors: A. Emerson, A. Grottesi, N. Spallanzani, F. Affinito
Guest Speaker: Massimiliano Bonomi (Univ. Cambridge)

AGENDA

September 28th 2016

09.30 – 10:15 *Registration*
10.15 - 11.00 *Introduction to HPC architectures (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 *Molecular Dynamics: Atom, Force and Domain Decomposition (A. Emerson)*
15.15 - 15.30 *Coffee break*
15.30 - 17.30 *Tutorial T1: Unix environment @ CINECA: modules, job scripts, PBS (N. Spallanzani)*

September 29th 2016

09:30 – 10:15 *Running MD on Hybrid HPC Architectures (A. Grottesi)*
10:15 – 11:00 *Tutorial T2: MD @ CINECA: script and benchmarks (A. Grottesi/N. Spallanzani)*
11:00 – 11:30 *Coffee Break*
11:30 – 12:30 *Tutorial T3: Scalability tests for biological systems (A. Grottesi/N. Spallanzani)*
12:30 – 14:00 *Lunch break*
14.00 - 15.00 *Tutorial T4: Analysis of MD trajectories: Essential Dynamics (A. Grottesi)*
15.00 - 15.30 *Coffee break*
15.30 - 17.30 *Tutorial T5: Running and analysing GROMACS and NAMD on a GPU/Xeon Phi cluster (A. Grottesi)*

September 30th 2016

9.30 – 12.30 **PLUMED Session: Talk and Tutorial**
9.30 - 10.15 *“Metainference Metadynamics with PLUMED”, (Massimiliano Bonomi)*

10.15-10.45 *Break*

10.45-12.30 *Hands-on tutorial.*

12.30 - 14.00 *Lunch break*

14.00 - 15.00 *Basics of ab. initio molecular dynamics (F. Affinito)*

15.00 – 15.30 *How to apply for computer resources from Cineca and PRACE (A. Emerson)*

15.30 -17.00 *Practical session or FREE*

** PATC course supported by the European Project PRACE-4ip. All lessons will be held in English.*