Efficient use of Molecular Dynamics simulation applications in an HPC Environment

17-19 November 2014- CINECA - BOLOGNA

PRELIMINAR AGENDA

Day 1 (17 Nov)

9.30 - 10.00 Registration and Welcome

10.00 - 11.00 Lesson 1. Introduction to HPC architectures

11.00 - 11.30 Break

11.30 - 12.30 Lesson 2. Introduction to Classical Molecular Dynamics

12.30 - 14.00 LUNCH

14.00 - 15.00 Lesson 3. Parallel Molecular Dynamics: Atom, Force and Domain decomposition

15.00 - 17.30 Tutorial T1. Analysis of a simple parallel program.

Day 2 (18 Nov)

9.30 - 10.30 Lesson 4.Running MD on HPC architectures I. Clusters and Hybrid clusters.

10.30 - 11.00 Invited Talk 1. (R. Gnudi, Uni. Modena) Porting of an MD code on Xeon PHI.

11.00 - 11.30 Break

11.30 - 12.30 Invited Talk 2. (I. Eberini, Uni. Milano). Simulation of urea-induced protein unfolding: a lesson from bovine β-lactoglobulin

12.30 - 14.00 LUNCH

14.00 - 15.00 Tutorial T2. Running and analysing Gromacs on a GPU cluster.

15.00 - 17.30 Tutorial T2. continued

Day 3 (19 Nov)

9.30 - 10.30 Lesson 5. Running MD on HPC architectures II. Bluegene/Q.

10.30 - 11.00 Tutorial T3.

11.00 - 11.30 Break

11.30 - 12.30 Invited Talk 3. PLUMED, (Giovanni Bussi, SISSA)

12.30 - 14.00 LUNCH

14.00 - 15.00 Lesson 6. A guide for accessing computer resources from funding bodies such as PRACE.

15.00 - 17.30 Q&A or FREE