

Material Science codes on innovative HPC architectures: targeting exascale

04-06 December 2017 – CINECA Casalecchio di Reno (Bologna)

*** Monday 4

- 09.00-09.30 Reception and introduction (F. Affinito)
- 09.30-10.30 HPC trends towards exascale and material science challenges (F. Affinito)
- 11.00-12.30 Introduction to CINECA HPC infrastructure (F. Affinito, A. Marani)
- 14.00-15.30 Yambo: introduction to the code (A. Ferretti)
- 16.00-17.30 Yambo: HPC exploitation, a test case (A. Ferretti)

*** Tuesday 5

- 09.30-10.30 Quantum ESPRESSO: introduction to the code and parallelization schema (P. Bonfà)
- 11.00-12.30 Quantum ESPRESSO: HPC exploitation, a test case (TBC)
- 14.00-15.30 GPU acceleration of plane-wave codes using SIRIUS library (A. Kozhenikov)
- 16.00-17.30 QE-GPU: an experience of porting to GPUs (Anoop Kaithalikunnel)

*** Wednesday 6

- 09.30-10.30 The AiiDA platform for computational materials science (A. Marrazzo)
- 11.00-12.30 AiiDA from a user's perspective: HPC and HTC stories (A. Marrazzo)
- 14.00-15.30 Opportunities from Accurate and Efficient Density Functional Theory Calculations for Large Systems (L. Genovese)
- 16.00-17.30 Electronic structure calculations in HPC framework: Solutions for profiling, load-balancing and post-processing (L. Genovese)