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Application porting and web services for the Molecular and Materials Sciences and Technologies community

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The increasing availability of computer power on Grid platforms has prompted the implementation of complex computational codes on distributed systems and, consequently, the development of appropriate visual interfaces and tools able to minimize the skills requested to the final user to carry out massive Grid calculations. In the present work we analyse the procedures adopted to implement on the infrastructure of the Italian Grid Initiative (IGI) some computational chemistry codes making use of the IGI web portal. The applications described here are those considered as use cases during the Italian Grid Training Workshop held in Rome in January 2014: CRYSTAL (ab initio quantum chemistry for calculations on crystals, slabs and polymers), Quantum Espresso (electronic structure and materials modeling atthe nanoscale) and VENUS (chemical dynamics for classical trajectory simulations). The three use cases cover the key situations met when running computational Molecular and Materials Sciences and Technologies applications on distributed computing infrastructures (DCI) and in particular High Throughput Computing, MPI runs and Distributed Data Management.

Wider impact and conclusions

The porting of legacy applications onto the Grid infrastructure, together with the development of the related gateways and related services, is being carried out as part of a more general effort to build a solid platform to be offered to the user as a service. The solutions designed and adopted in the present work enable the user to perform computational studies by making use of proper configured DCIs where inner complexity has been masked and the best strategies aimed at saving time and computing resources can be devised. Moreover, the distributed data management mechanism implemented in the portal allows a deep control of the data stored in the distributed environment and an easy handling between distributed and local resources. The implemented applications and related case study provide a reusable example for other communities interested in porting their applications to production Grid systems.

Description of work

We have ported on the grid environment a set of computational chemistry applications and make them easily accessible using the IGI web portal.
The applications chosen for that purpose and making use of the IGI resources available to the GRIDIT and COMPCHEM VOs, are:
- CRYSTAL (http://www.crystalsolutions.eu/crystal14-released.html), is a quantum chemistry ab initio program designed for calculations on crystals, slabs and polymers using translational symmetry written at the University of Torino (IT) and the Computational Materials Science Group (Daresbury, UK). The current version is CRYSTAL14 that was released on December 2014 and requires parallel resources (MPI) and long time simulation runs.
- Quantum Espresso (www.quantum-espresso.org), is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale maintained by the homonymous foundation and based on density-functional theory, plane waves, and pseudopotentials. It requires parallel resources and long time simulation runs.
- VENUS, is a open source code developed at the Texas Technical University (Lubbock, US) for general chemical dynamics classical trajectory simulations making use of analytic functions to represent the potential energy surface (PES) for the chemical system. Each calculation is independent making the code suited for and HTC approach.
The three codes have been compiled reflecting their computational needs and specific web GUIs have been designed to tackle the following important aspects:
- an automatic checkpointing mechanism has been developed and implemented in the web GUI. The mechanism supports also for Quantum Espresso the automatic resubmission of the job.

- an automatic check of the evolution audit of the calculations at runtime has been implemented as a facility that exploits Grid Storage Elements, to make temporary files and partial output available for runtime inspection.

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