Contribution ID: **60** Type: **Oral**

Porting of Computational Chemistry legacy applications on the EGEE Grid platform: computational aspects and visualization tools

Tuesday, April 13, 2010 11:00 AM (20 minutes)

The work carried out to implement complex computational chemistry suites of codes on distributed systems and, at the same time, to develop appropriate graphical tools for the visual rendering of the outcomes of the calculations on the production EGEE Grid infrastructure available to the COMPCHEM VO, is here presented and discussed with some examples.

Detailed analysis

To this end the ABC code has been ported into the EGEE Grid environment using the P-GRADE Grid Portal. It has also been complemented with relevant visualization tools.
ABC is a quantum mechanical atom-diatom reactive scattering program that carries out accurate calculations of the quantum S matrix elements to evaluate reaction probabilities as well as state-to-state integral and differential cross sections.
Typically, ABC can be executed several times for different sets of input parameter values, consuming a large amount of CPU hours and collecting large amounts of output data. The visual analysis of the output files carried out by the procedure has been greatly improved with respect to that of the standard P-GRADE version using a set of java based graphical tools implemented as standard pluggable user interface components called Portlets. The final user can in this way compare the outcomes, with no need to download all the output files which remain on the server, and evaluate the possible strategies for a new calculation.

Conclusions and Future Work

The porting of legacy computational chemistry applications onto the Grid infrastructure, together with the development of the related visualization tools, is being carried out as part of a more general effort to build a solid platform for assembling accurate multi scale realistic simulations and for establishing an advanced molecular and material science research environment.

Impact

The increasing availability of computer power on Grid platforms has become a strong incentive to implement complex Computational Chemistry suites of codes on distributed systems and to develop appropriate distribution models. On this ground the Virtual Organization (VO) COMPCHEM assembled out of a group of molecular and material sciences laboratories committed to implement their computer codes on the EGEE production Grid infrastructure is building a library of molecular dynamics codes to be offered to its users as services including not only the concurrent production of the numerical results but also related graphical rendering.
The implemented case study demonstrates the possibility to reuse the present porting process in order to provide a reusable example for other groups which are interested in porting their applications to production Grid systems.

Keywords

Computational Chemistry, application porting, visualization tools

URL for further information

http://compchem.unipg.it

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Session Classification: Computational Chemistry

Track Classification: Experiences from application porting and deployment