Contribution ID: **57** Type: **Poster**

Porting of a Quantum Mechanics Reactive Scattering Program on the Grid infrastructure

Tuesday 23 September 2008 16:31 (1 minute)

Describe the activity, tool or service using or enhancing the EGEE infrastructure or results. A high-level description is needed here (Neither a detailed specialist report nor a list of references is required).

The goal of the COMPCHEM VO is to implement complex computational chemistry suites of codes on distributed systems and to develop appropriate distribution models on the production EGEE Grid infrastucture. More specifically, the goal of implementing grid empowered versions of quantum reactive scattering codes dealing with atom-diatom systems can be seen as part of a more general effort to design suitable distributed workflows for the ab initio simulation of molecular systems.

Report on the impact of the activity, tool or service. This should include a description of how grid technology enabled or enhanced the result, or how you have enabled or enhanced the infrastructure for other users.

The use of P-GRADE Grid Portal permitted us to define and to execute the ABC code as a parameter study application on the EGEE Grid. Due to the fact that each simulation can run independently from the others (the program is executed on multiple grid resources with different input files simultaneously), distribution may involve a large area network of computers.
In our study case the different ABC jobs work with different "Maximum rotational quantum"and "Maximum hyperradius"values in a typical search for convergence. These values (jmax and rmax) are stored in the same input file along with other input parameters of the simulation.
As a matter of fact in our bench runs we measured between 2 and 4 times faster execution on the grid than on a local machine.
A better performance and higher speedup can be achieved on the Grid if more parameter study jobs are executed within a single grid execution.

Describe the added value of the grid for your activity, or the value your tool or service adds for other grid users. This should include the scale of the activity and of the potential user community, and the relevance for other scientific or business applications.

The ABC quantum mechanical atom-diatom reactive scattering program has been ported on the EGEE Grid. ABC 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 and has a larege CPU demand. The ABC porting has been carried out with the help of the Grid Application Support Centre (GASuC) using the open source tool called P-GRADE Grid Portal that provides intuitive graphical interfaces and does not require the modification of the code to execute it on a Grid platform. The gridification process permitted us to evaluate the possibility

of collecting spare cycles for ABC simulations from the COMPCHEM VO of EGEE.
Moreover, several computational chemists who would be interested in the execution of the code are members of the COMPCHEM VO and this means hat they can share the application and execution results on the common EGEE Grid platform.

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Session Classification: Demos and Posters

Track Classification: Poster