Contribution ID: **118** Type: **Oral**

Parallel Execution of Chemical Software on EGEE Grid

Wednesday, February 13, 2008 4:00 PM (30 minutes)

The current state of development of grid middleware allows easy parallel execution in case of software using any of MPI flavour. Unfortunately many chemical packages do not use MPI for parallelization therefore special treatment is needed. Gaussian can be executed in parallel on SMP architecture or via Linda. These require reservation of certain number of processors/cores on a given WN and the equal number of processors/cores on each WN, respectively. The current implementation of EGEE middleware does not offer such functionality therefore the only solution is to enforce required configuration via Maui scheduler. The solution we present does not require Linda for parallel execution. It allows utilization of maximum number processors/cores on a given WN. Taking in to consideration the WNs supporting Gaussian VO parallel execution on maximum 8 processors/cores is possible. The main disadvantage of our solution is necessity of local Maui configuration on each site by an administrator.

Provide a set of generic keywords that define your contribution (e.g. Data Management, Workflows, High Energy Physics)

parallel execution, commercial software, license issues

4. Conclusions / Future plans

The grid port of the parallel version of Gaussian package has been developed to fulfil community needs especially for large molecular system studies as easy for use as the serial version was in the past. At the same time we have demonstrated the possibility of execution of parallel versions of chemical software on the grid even if the middleware does not support the parallelization model directly. Our future work will focus on other parallel versions of packages as required by the community.

3. Impact

The port of parallel version of Gaussian packages on the grid has been shown as a next step towards better grid utilization and better community satisfaction. As the simplicity of the usage of the parallel version of the software on EGEE Grid remains unchanged we expect a quick switch to the usage of the parallel version of the software not only in case of Gaussian but also for other packages like NAMD, GAMESS or Turbomole for which parallel versions have been ported to the grid recently. It is also important to note that our solution may serve as a prototype for other difficult cases where there is no direct support for specific parallel execution model by the middleware.

URL for further information:

http://egee.grid.cyfronet.pl/gaussian

1. Short overview

Constant interest among chemical community to study larger and larger molecules forces the parallelization of existing computational methods in chemistry and development of new ones. These are main reasons of frequent port updates and requests from the community for the grid ports of new packages to satisfy their computational demands. Unfortunately some parallelization schemes used by chemical packages cannot be directly used in grid environment. Here we present a solution for Gaussian package.

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Session Classification: Workflow and Parallelism

Track Classification: Application Porting and Deployment