Contribution ID: **117** Type: **Demonstration**

Utilization of EGEE Grid as a Computational Platform for Chemistry

Tuesday, February 12, 2008 4:00 PM (0 minutes)

A huge amount of work has been devoted to satisfy chemical community requirements on the grid. The activity of CompChem, Gaussian and VOCE VOs has been mainly focussed on the grid ports of chemical software packages and on the development of grid tools that simplify job manipulation and workflows, automating complex data management tasks. The ports targeted commercial software packages like Gaussian, Turbomole or Wien2k, in particular as the community is highly accustomed them. The main difficulty concerned licenses for which grid solutions had to be developed. In parallel, grid ports of other packages for ab initio, molecular dynamics and quantum dynamics (including time) has been developed mainly for the GEMS project. The development in job management resulted in the Charon Extension Layer, the latest version of which allows easy job manipulation via a web browser. Workflows are mainly available to the Wien2k and GEMS communities to solve their complex data submission issues.

3. Impact

The availability of variety of above mentioned software packages on the grid resulted in their application to many areas of computational chemistry including chemical reactions studies like N+N_2 or Cl+CH_4 with help of very accurate ab initio and quantum dynamics methods, modelling of catalytic centres and possible reaction paths to understand the way active centre interacts with substrates and products, analysis of ions flowing through a carbon nanotube to later apply similar models for ions transfer through molecular membranes or attempts of charge transfer modelling between carotenoids and chlorophyll during photosynthesis process. The EGEE grid utilization by these applications place computational chemistry on third position just after HEP and Biomed. Also, it is worth noting that other communities like solid state physics, pharmacy or climate are interested in usage of chemical packages.

If demonstration is requested please explain what visual or interactive aspects of the contribution necessitate a demonstration rather than a presentation or poster?

The demonstration will show the important aspects of chemical computations on the grid along with scientific results obtained on the it. We will also focus on new futures, which will be available for chemist in a near future. To demonstrate this a network connection to present preliminary achievements will be necessarily. Finally we'll present guidance for user to help them better plan the computations to maximize benefits form grid usage.

URL for further information:

http://compchem.unipg.it; http://egee.cesnet.cz/en/voce; http://egee.grid.cyfronet.pl/gaussian

4. Conclusions / Future plans

The chemical software ports, easy job handling systems and use of workflows to manage complex data resulted in numerous applications ported to the grid infrastructure. We have also enabled chemical software for other communities and we are working now to make software ported by these communities available for chemists. Our future work will include further development of grid license models and web portal with software plug-ins to enable the grid platform for non-expert users.

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

computational chemistry, license issues, commercial software, software porting

1. Short overview

The current focus of computational chemistry far exceeds the traditional interest of studying properties of small molecules. Fast development of new materials like polymers or drugs not only requires numerous applications of computational chemistry methods to study their properties but also helps to design new materials with desired properties. Such simulations demand however, huge computational resources. Thus a grid platform can be seen as one of the answers to these demands.

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Session Classification: Demonstrations

Track Classification: Scientific Results Obtained Using Grid Technology