5th EGEE User Forum

Contribution ID: **94** Type: **Demonstration**

Grid Web Portal with software plug-ins to chemical software

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New users, especially those accustomed to Graphic User Interfaces (GUI), often face difficulties during the adoption of grid computing for the research. The main source of issues is related to command line interfaces which are hard to adopt by non-experts. To avoid users'disappointment a new web based interface has been proposed. In contrast to existing web-based tools the portal developed facilitates not only job management but primarily can serve as a work environment for chemists. Here, we present the current status of the portal development including several plug-ins to first principles chemistry packages.

Detailed analysis

Existing web portals focus mainly on tasks, which simplify job management on the Grid. Although this is very important, this part of portal functionality is not sufficient for scientists accustomed to GUI environments supporting their research conduction. Our solution, in contrast to other existing web portals, is "user centric" instead of "grid centric". Therefore, it provides tools facilitating research conduction and "hides"the existing grid infrastructure from the user as much as possible. The tools adopted in the portal, based on ViroLab Project technology together with Google Web Toolkit library, allow for easy planning, development and execution of complicated computational experiments without being distracted by the grid technology. Currently users can execute and modify the existing experiments allowing execution of Gaussian, Turbomole and GAMESS US packages including a variety of computational chemistry methods. Other tools integrated in the portal allow an analysis of the results of computational experiment(s) (energy for example) and their visualization. Particular experiment results can be displayed via external software.

Conclusions and Future Work

The Grid web portal for chemists has been developed to fulfill community needs especially coming from users newly adapting to the Grid. Although the number of software packages supported by the portal is still limited, the collection of computational methods provided by the above software suites allows studies of a variety of molecular properties at various levels of accuracy. Nevertheless, our future work will focus on the adoption of other packages to extend the available portfolio, as well asthe integration of the portal with national grid infrastructures for the benefit of their users.

Impact

The development of grid web portal for chemists is a next step towards better community satisfaction. As it focuses on computational experiments in chemistry rather then job management only, we expect high interest in it, coming mainly from new users adopting the EGEE Grid. The availability of the portal will not only avoid new users'disappointment but what is more important will drastically shorten the time needed for the adoption of grid computing to particular computational problems in chemistry. Although the current version is limited to the several first principles codes only, most of the important chemistry tasks like chemical reaction paths, potential energy surfaces, or even ab initio molecular dynamics studies, can be easily performed onthe EGEE infrastructure.

Keywords

web portal, software plug-ins, computational chemistry software

URL for further information

Under construction. Probable address: http://chempo.grid.cyfronet.pl/chempo

Justification for delivering demo and/or technical requirements (for demos)

A demo offers possibility to reach much broader audience than during ordinary session. No special requirements is required – a tv screen and fast internet connection for live demonstration

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Session Classification: Demo Session 1, Welcome Drink

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