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Current status of Chempo web portal

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Abstract

New Grid users often face difficulties when using command line interfaces. This makes their adoption in the Grid environment much harder. To avoid users'disappointment, new web-based interface is proposed. In contrast to the existing web based tools the proposed portal will not only facilitate job management but primarily will serve as a work environment for chemists. Here, we present the current status of the portal development with particular focus on plug-in to the Gaussian computational chemistry package.

Existing web portals focus mainly on tasks, which simplify job management on the Grid. Although this is a 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, our aim was to provide tools facilitating research conduction and "hide"the existing grid infrastructure from the user as much as possible. The tools based on ViroLab Project technology together with Google Web Toolkit allow for easy planning, development and execution of computational experiments without being distracted by the grid technology. Currently users can execute and modify the existing experiments or create new ones with the help of the Gaussian package. Other packages will be incorporated in the near future.

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 on the EGEE Grid. The availability of the portal will not only avoid new users'disappointment but what is more important will drastically shorten time needed for their adoption to the grid. Although the current version is limited to the Gaussian package only, most of the important chemistry tasks like chemical reaction paths, potential energy surfaces or even ab initio molecular dynamics can be easily performed on EGEE infrastructure.

The Grid Web portal for Chemists has been developed to fulfill community needs especially coming from users newly adapting to the Grid. Although number of software packages supported by the portal is very limited the collection of computational methods provided by Gaussian suite allows studies of variety of molecular properties. Nevertheless, our future work will focus on further adoption of other computational chemistry packages to extend available portfolio.

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