Contribution ID: **39**   Type: **Poster**

DrugScreener-G: An Integrated Environment for Grid-based Large-Scale Virtual Screening and Drug Chemical and Bio-macromolecule Modeling

Tuesday 23 September 2008 16:20 (1 minute)

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.

With the recent great success of the WISDOM application, research about virtual screening methods using Grid computing attracted much attention of not only researchers involving in drug discovery and development, but also those seeking applications of Grid computing. DrugScreener-G will make the Grid-based large-scale virtual screening easily reproducible for users and enhance its productivity. It will also provide biologists and bioinformaticians without much knowledge of Grid computing with easy-to-use tools for a more friendly approach of Grid-based large-scale virtual screening.

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.

DrugScreener-G will help users in drug discovery, biochemistry and biology to access the EGEE infrastructure and exploit its full power in drug discovery and virtual screening without serious efforts to learn the EGEE middleware commands and tools. The scope of user community who may be benefitted by using DrugScreener-G spans from drug chemists to biochemists and biologists for whom large-scale screening gives any insight and added value to their research. Tools and components discovered during the development of DrugScreener-G, such as credential management plug-in, application repository, parametric sweep study plug-in, Grid interoperability plug-in based on GIN, SAGA and meta-schedulers, are expected to be utilized in other application software using the EGEE infrastructure and Grid computing. DrugScreener-G is also expected to be a sound example of a scientific application software seamlessly and effectively utilizing cutting-edge cyber infrastructure of Grid computing.

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).

DrugScreener-G is an integrated environment for virtual screening, which implements the basic ideas of Grid-based large-scale virtual screening of the WISDOM project into a concrete software. DrugScreener-G is easily extensible with plug-in-based architecture and hides details of Grid computing from users by using web

service in communications with the WISDOM Production Environment to manage and perform the docking simulations on the EGEE infrastructure, and to get the results back to the users.

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Session Classification: Demos and Posters

Track Classification: Poster