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An Intuitive Web Interface for Massive Molecular Docking on the Grid

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Describe the scientific/technical community and the scientific/technical activity using (planning to use) the EGEE infrastructure. A high-level description is needed (neither a detailed specialist report nor a list of references).

The avian flu data challenge in last spring has successfully demonstrated a high-througput docking service on the EGEE infrastructure. The next step is to make this service more accessible to real biology end-users rather than grid specialists. Collaborating with biomedical researchers, we have developed an intuitive web interface for biologists to access the massive molecular docking service on the EGEE infrastructure.

Report on the experience (or the proposed activity). It would be very important to mention key services which are essential for the success of your activity on the EGEE infrastructure.

This work is built on top of the DIANE framework. DIANE was originally developed for handling the distributed applications within a Master-Worker model. It provides an overlay system on top of the Grid system, in which the pull-mode scheduling and failure recovery mechanisms are implemented based on the CORBA protocol. On the other hand, the DIANE framework hides the details of the job operations on the Grid so that application developers can concentrate on the implementation of application logic and interface design. DIANE interfaces the EGEE infrastructure through a high-level grid tool, GANGA (http://cern.ch/ganga).

With a forward look to future evolution, discuss the issues you have encountered (or that you expect) in using the EGEE infrastructure. Wherever possible, point out the experience limitations (both in terms of existing services or missing functionality)

As the efficiency of the grid-enabled docking service has been demonstrated by the data challenge, we expect a well customized interface can encourage biology researchers to use the service for their daily research. In developing the web interface, we experienced that adopting high-level Grid application frameworks (e.g. DIANE and GANGA) can dramatically reduce the effort in handling Grid jobs, concerning the work of failure recovery, and of application specific monitoring and bookkeeping.

Describe the added value of the Grid for the scientific/technical activity you (plan to) do on the Grid. This should include the scale of the activity and of the potential user community and the relevance for other scientific or business applications

Aiming at making the grid-enabled docking service more useful for biologists, we developed a web-based user interface on top of the DIANE framework (http://cern.ch/diane), trying to reduce researchers'effort in accessing the service and in analyzing the docking results. By hiding the technical details, the interface exposes only the configurations meaningful for biologists. Through this interface, biologists could set a filter on a compound library and select interesting targets and ligands by visually examining their structures. Leveraging on the interactive feedback feature of the DIANE framework, results of finished dockings are not only ranked in table; they are also transformed into 3-D structures so that biologists can immediately look into the docking poses and download corresponding results to their local disk for further analysis.

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