Contribution ID: **5** Type: **Demo**

Grid-enabled virtual screening service based on grid application platform

Tuesday 23 September 2008 16:00 (1 minute)

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).

The first and second grid challenges preparing for avian flu drug discovery in mutations have demonstrated that the biomedical communities can be largely benefited from the EGEE infrastructure in terms of the speed and the reaction time of screening over a full spectrum of the compound libraries. Based on Grid Application Platform, the grid-enabled virtual screening service has been proved to be very useful to increase the hit rate, reduce the cost and shorten the time to biomedical activities.

Abstracts for online demonstrations must provide a summary of the demo content. Places for demos are limited and this summary will be used as part of the selection procedure. Please include the visual impact of the demo and highlight any specific requirements (e.g. network connection). In general, a successful demo is expected to have some supporting material (poster) and be capable of running on a single screen or projector.

The demo will show a grid-enabled virtual screening service which is a customized GUI application used by biology users, through the friendly GUI, who can easily run their docking simulation jobs on the EGEE infrastructure.

Therefore, In the demo, a completed virtual screening process will be demonstrated, a real-life job containing about 1000 docking simulations (~6000 minutes CPU time) will be prepared and executed.

We will also demonstrate how users can perform the job management and the visualization of the simulation results through the GUI. Thereafter, one advanced refinement simulation will also be demonstrated.

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.

GAP makes use of DIANE to distribute docking simulations on the grid. The DIANE has the features providing agent-based task pulling model with high-level failure recovery mechanism to ensure a steady job throughput. Therefore, the system can also distribute the computing jobs in available grid resources by running multiple DIANE instances.

Those distributed DIANE instances are integrated by a Virtual Queuing System, the high level job manager of the Grid Application Platform developed by ASGC. Through it, users can manage the distributed DIANE instances as controlling jobs in a job queuing system.

Those essential information from the simulation results are stored in the AMGA catalogue system as the metadata. The user can analyse the aggregative datas through the AMGA queries rather than looking into the results widely distributed on the grid storage elements.

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.

The grid infrastructure is an integrated environment providing "on-demand"resources for the compound-protein docking simulation. A grid service of virtual screening was developed to better leverage the underlying grid infrastructure and hide complexity from the users. Domain experts thus could focus on scientific workflow and analysis without caring too much on the grid system and service operations. We developed and deployed the drug discovery system is not only providing the grid-enabled computing simulation but also representing an emulation workflow of the wet-lab screening based on the processes(initial screening, filtering and refinement screening). Through this system, users can have grid-enabled virtual screening service in running the docking simulation, visualizing the whole simulation process and managing the results on the grid environment. Biochemists would focus on the composition and re-purposing grid services to reach the best effective analysis workflows on GAP.

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