

## **Grid-enabled Virtual Screening Service based on Grid Application Platform**

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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 (GAP), 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.

GAP makes use of DIANE to distribute docking simulations on the grid. 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.

For the current status, we have upgraded DIANE1 to DIANE2. DIANE2 has more capability to handle more workers, which makes this Grid-enabled virtual screening service could have better performance in terms of finishing the massive docking simulation tasks.

We introduce a user-friendly graphical user interface desktop application for using this Grid-enabled virtual screening service. Through the GUI, the end-users can easily take the advantage from GRID for large-scale virtual screening. Furthermore, they can even upload their own target and ligands, and do the same docking process, visualization and analysis with this GUI, of course including the advanced refinement

docking simulations. The end-users can finally have a real GRID-enabled desktop utility for the virtual screening service for their daily research.