

Integrate Virtual Screening Service with Desktop Grid by DeGISCO infrastructure

To make the high throughput large-scale molecular docking running the grid infrastructure, ASGC developed the GVSS (GAP Virtual Screening Service) application package that incorporates the EGEE gLite middleware. This is a Java-based graphical user interface application specifically developed for drug discovery service. Users can use the complex computing resources of grid for screening by only selecting the proteins and ligands, and visualize the docking results by the graphical interface. Traditionally, the Computing Elements (CE) of Service Grid (SG) are established by research institutes on the world-wide grid computing infrastructure. In recent years, there is another type of grid computing resources which use the desktop computers as shareable computing resources called Desktop Grid (DG). One of the representative DG infrastructures of built on using the BOINC which was developed by University of California, Berkeley. Because of the service architecture's differences, the resources of SG and DG were not sharable. Since 2008, EDGeS project which was initiated by European Union is committed to integrate of SG and DG. This project developed 3G - Bridge as its intermediary service to bridge the two services. After the end of the two years project, the succeeding DeGISCOproject continues to develop the 3G-Bridge, and promotes this infrastructure to more institutes to port applications across SG and DG. Since the middle of 2010, we participated in DeGISCOproject and began to integrate GVSS with 3G-Bridge technology, expecting scientists who engage in drug discovery will be able to utilize more computing resources through GVSS.

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