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Grid-enabled virtual screening service against the epidemiological disease

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GAP Virtual Screening Service (GVSS), a large-scale in-silico drug virtual screening service, provides a system to speed-up the searching process among all conformations of a compound. Moreover, GVSS is a generic drug discovery framework over gLite by which users can upload their compounds and targets to do grid docking, compare the significance, and verify results by in vitro experiment afterwards. GVSS has proved to provide intensive computing power and effective data management over gLite infrastructure on neglected and emerging diseases, such as Avian Influenza and Dengue Fever.

Detailed analysis

In the study of Biomedicines, the structure based molecular docking simulation is a common method for predicting potential interacting complexes of small molecules in protein binding sites. However, Massive molecular docking required intensive computing power and effective data management. A GRID computing framework was established for AutoDock 3.0.5 and evaluated for its quality of large-scale molecular docking process. GRID is an ideal environment, which can provide large-scale and on-demand resources, including computing and storage resources.

GVSS is a user-friendly graphical user interface enhanced desktop application for using this Grid-enabled virtual screening service. Through the GUI, the end-users can easily take advantage of GRID computing resources 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 drug docking scientific gateway, 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.

Conclusions and Future Work

To enhance the in silico pipeline processing for the application, we use another more accurate molecular simulation package APBS (Adaptive Poission-Boltzman Solver) in conjunction with the Autodock results. Furthermore we expect to foster the biomedical grid activities and promote the e-Science collaboration between partners in Asia and Europe.

Impact

Inspired by the successful experiences on Avian Flu Data Challenges, ASGC developed the GVSS application package that incorporates the EGEE gLite middleware DIANE2 and AMGA. Therefore, ASGC coordinated the Dengue Fever Data Challenge via EUAsiaGrid VO in June 2009. The objective was to utilize the grid enabled high throughput screening for structure–based computational methods to identify small molecule protease inhibitors. 300,000 compounds from the ZINC CDI compound library, a free database of commercially available compounds, were selected for virtual screening.

For this activity, we allocated 268 CPU-cores computing resources from EUAsiaGrid partners including Taiwan, Thailand, Vietnam, MIMOS Malaysia, UPM Malaysia and CESNET. For the phase I, a total of 46 GB of data from execution of the 300,000 jobs were generated.

Keywords

Grid Applications, Drug Discovery, Virtual Screening, Avian Influenza, Dengue Fever, Epidemiological

URL for further information

http://gap.grid.sinica.edu.tw

Author: Mr CHEN, HsinYen (Academia Sinica Grid Computing)

Co-authors: Mr YEN, Eric (Academia Sinica Grid Computing); Dr LIN, Simon (Academia Sinica Grid Computing)

Presenter: Mr CHEN, HsinYen (Academia Sinica Grid Computing)

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