Virtual Screening Service based on Grid Application Platform

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Grid Application Platform was developed by ASGC. And enabling grid support for virtual screening service based on Grid Application Platform(GAP) was developed and can make virtual screening service use large-scale and on-demand resources which can shorten the response time to emergency disease.

The system uses DIANE to distribute docking simulations on the grid. DIANE features an agent-based task pulling model with high-level failure recovery mechanism to ensure a steady job throughput. And the distributed DIANE instances are organized by a Virtual Queuing System, part 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.

Essential information from the simulation results are stored in the AMGA catalogue system as the metadata. Aggregative data analysis could be done easily by AMGA queries rather than looking into the results widely distributed on the grid storage elements.

Short overview :

Grid Application Platform short for GAP, is a layered framework which aims to reduce the efforts of porting applications to the Grid, and also aims to make an intuitive user interface which is light-weight, portable and cross-platform client for end users.

Screening is the first measure to take for the biological activity of each compound in a large compound collection against an disease target. And Virtual Screening is a computer-based simulation for screening, Virtual Screening using the Grid through GAP can have large-scale and on-demand resources which can shorten the response time to emergency disease.

Impact :

Developers can reduce many routines and tedious works and reuse these efforts through GAP. And no more low-level commands or services will directly face to the end users, instead of using the system with the highly abstracted functions.

Conclusions :

According to our ideas, the grid-enabled application will have large-scale and on-demand resources for the virtual screening service, one instance based on GAP, and the biologists will have a productive system

enabling them to run docking simulations and to manage the docking results on the grid as simple as using a desktop utility in the daily research.