Contribution ID: **47** Type: **Demonstration**

DrugScreener-G: Towards Grid-enabled Large-Scale Virtual Screening Coming into Handy

Monday 12 April 2010 17:10 (10 minutes)

DrugScreener-G (DSG) is an intuitive and easy-to-use grid-enabled in silico screening tool, aiming to help scientists in drug discovery including biologists and biochemists to conduct a large-scale deployment of virtual screening process on the Grid. With the help of DSG, scientists can easily have access to the PDB database, download and view the 3D structure of target proteins of interest, launch and manage millions of protein-ligand docking simulations on the Grid. To facilitate the analysis of docking results, visualization tools like Jmol and Chimera have been integrated into DSG as well.

Detailed analysis

DSG was developed based on client/server architecture. The DSG server takes care of details of the complexity of Grid-related operations including maintaining thousands of agents distributed on the Biomed VO of EGEE that actually perform the docking simulations. Indeed, it is quite challenging to get millions of in silico dockings done on the public Grid infrastructure like EGEE as it requires the grid-relevant issues of scalability, performance and fault tolerance to be seriously addressed. The DSG server was implemented as a web service that has adopted, as its core grid engine, the WISDOM Production Environment, a widely accepted grid-enabled virtual screening technology. The DSG client was developed as an Eclipse RCP-based application, providing an easy-to-use GUI interface for (1) preparing a set of ligands and target proteins by allowing accessing well-known public biological databases such as ChemBridge, ZINC and PDB database, (2) submitting docking simulation jobs to the Grid via the DSG server, (3) monitoring the progress of the simulation jobs, and (4) the post-processing of the docking results to help uncover their biological meaning.

Conclusions and Future Work

DSG is an easy-to-use integrated tool for scientists, who usually have a resistance to learning complicated yet powerful IT technologies like Grid computing, to harness the power of its production infrastructure to carry out large-scale in silico experimentation of their own. DSG has implemented some basic ideas of the virtual screening processes. In future versions, it will support (1) consensus docking by integrating multiple in silico docking tools (e.g., Flexx, Autodock, etc) and (2) multistep docking by supporting the execution of Molecular Dynamics (MD) simulations.

Impact

The WISDOM initiative, a large-scale deployment of virtual docking on production Grid infrastructures, has been seen in the EGEE community with great success from the scientific and grid deployment perspective. However, from the usability point of view, there seems to be a lot to be done in order to be able to get the grid-enabled in silico approach easier to use for non-experts of grid computing. DGS targets researchers and scientists in drug discovery, biology and biochemistry to help them have access to the Grid infrastructure and exploit its full power in drug discovery and virtual screening without having to learn details of grid middleware services and tools. DSG is expected to help them capture more insight into the grid-enabled approach to large-scale virtual screening and thus enhance their research productivity in drug discovery. The DSG client tool

is now being used and tested by biologists in Chonnam National University, one of long-time partners of the WISDOM collaboration. With the help of tools like DSG, their long-time dream of conducting large-scale virtual screening on their own at any time without any help from grid experts is to be made realized in the near future.

Keywords

virtual screeing, in-silico docking, grid-enabled, production grid, drug discovery

URL for further information

http://anakin.kisti.re.kr/DrugScreenerG

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Session Classification: Demo Session 1, Welcome Drink

Track Classification: End-user environments, scientific gateways and portal technologies