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DrugScreener-G: an Integrated Environment for Grid-enabled Large-Scale Virtual Screening with Tools for Computer-Aided Drug Design and Modeling

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DrugScreener-G is an integrated environment for virtual screening, which implements the basic ideas of Grid-enabled large-scale virtual screening of the WISDOM project into a concrete software. DrugScreener-G is easily extensible with plug-ins. DrugScreener-G hides details of Grid computing from users by using web services in communication with the WISDOM Production Environment to manage and perform the docking simulations on the EGEE infrastructure, and to get the results back to users.

Impact

DrugScreener-G will help users in drug discovery, biochemistry and biology to access the Grid infrastructure and exploit its full power in drug discovery and virtual screening without making serious efforts to learn the Grid middleware commands and tools. The scope of the user community who may benefit from using DrugScreener-G spans from drug chemists to biochemists and biologists for whom large-scale screening gives any insight and added value to their research. DrugScreener-G is expected to be a sound example of a scientific application seamlessly and effectively utilizing cutting-edge cyberinfrastructure of grid computing. DrugScreener-G will make the Grid-enabled large-scale virtual screening easily reproducible for users and enhance their productivity. It will also provide biologists and bioinformaticians without much knowledge of Grid computing with easy-to-use tools for a more friendly approach to Grid-enabled large-scale virtual screening.

URL for further information

http://anakin.kisti.re.kr/trac/DrugScreenerG (tentative, not yet available fully)

Conclusions and Future Work

DrugScreener-G is an easy-to-use integrated environment for non-experts of Grid computing to utilize the full power of Grid computing for virtual screening. In future versions it will support consensus docking and multistep docking with workflow support. R language client will be supported for post-processing and automated analysis of the virtual screening results. It will also integrate Java-based advanced visualization and modeling tools for a more user-friendly interface.

Keywords

integrated environment, plug-in, Grid-enabled large-scale virtual screening, drug discovery

Justification for delivering demo and technical requirements (ONLY for demonstrations)

In last presentation of DrugScreener-G at EGEE'08 conference, the development of a prototype version of DrugScreener-G had been still going on to prove that its design concepts and architecture worked well. The

first prototype version of DrugScreener-G is now ready and we would like to show the prototype to EGEE users, to hear comments and feedback from users working for drug discovery. We also want to show how DrugScreener-G can enhance productivity in virtual screening with Grid computing.

Detailed analysis

We report the current status of DrugScreener-G development, requirements and features to be developed, related technologies, and future directions and prospects. Three important characteristics of DrugScreener-G, extensibility based on plug-in architecture, support for multiple methods of virtual screening in a single environment, and interoperability in application-level among different types of computing resources, are discussed. DrugScreener-G is easily extensible with new virtual screening schemes as it is based on plug-in-based architecture. With plug-ins for various docking applications and combinations of them into new plug-ins or a pipe-lined workflow with a workflow engine, DrugScreener-G can extend its capability to a new virtual screening method. To hide technical details of grid computing on the user's side and to provide interoperability among different types of computing resources, all of the Grid computing related operations are hidden under web services.

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