Contribution ID: **87** Type: **oral presentation**

Docking and Moleculardynamik - Complete 15 stage workflow with gLite WMS

Thursday 10 May 2007 09:40 (20 minutes)

Describe the scientific/technical community and the scientific/technical activity using (planning to use) the EGEE infrastructure. A high-level description is needed (neither a detailed specialist report nor a list of references).

Docking is the method of first choice for rapid in silico screening of large ligand databases for drug research, since it is based on a rational physical model and very fast. Thus, in 2005 during the first WIDSOM data challenge this method has been employed to screen the ZINC database for compounds potentially inhibiting the Malaria parasite plasmodium falciparum by blocking one of its particular proteases. As a result, guanidinium compounds, so far not known to inhibit the tested plasmepsin hav

Report on the experience (or the proposed activity). It would be very important to mention key services which are essential for the success of your activity on the EGEE infrastructure.

Therefore, a workflow combining the docking program FlexX2,3 and parts of the molecular dynamics (MD) package AMBER 84 has been set up. Since MD calculations tend to become quite consumptive, the workflow has been implemented using the EGEE-middleware gLite5 for performing world wide large scale studies in order to rerank the hits of the previous simple docking experiment. With the invention of the Workload Management Service gLite is able to handle so-called DAG (Directed Acyclic Graphs) jobs. Our directly with gLite features deployed workflow consist of 15 stages were each stage consist of subjobs and the number of subjobs depend on the size of the input. No portal and no workflow engine is used. Each stage executes the different programs like FlexX, Amber etc. Data is held on the storage elements and Metadata is stored in database.

With a forward look to future evolution, discuss the issues you have encountered (or that you expect) in using the EGEE infrastructure. Wherever possible, point out the experience limitations (both in terms of existing services or missing functionality)

We will present and first results generated during WISDOM2 for demonstrating both,
the benefits as well as the limits of the chosen approach. We will discuss also the
problems encountered with experiments, where a DAG Job, controlled by WMS starts
hundreds of follow up jobs automatically over many days and the dependencies on the
stability of the resources. It is of interest to run the Moleculardynamik part of the
workflow on DEISA. We are in discussion with FzJ to use it as Demo.

Describe the added value of the Grid for the scientific/technical activity you (plan to) do on the Grid. This should include the scale of the activity and of the potential user community and the relevance for other scientific or business applications

Drug design for neglected deseases is adressed in the WISDOMI and II.
The docking process is now combined with Moleculardynamics, which is heavy computing
intensive and may be provide more accurate results.

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Session Classification: Workflow

Track Classification: Workflow