Type: poster

## **Protein Clustering on the EGEE**

Wednesday 9 May 2007 17:30 (20 minutes)

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

As protein databases are growing up day after day, the clustering process on interesting datasets in a single machine is not feasible due to memory constrains. A Grid environment allows an adaptive database distribution in order to optimize its overall analysis. The complexity of the workflow inherent to "CD-HIT"needs a robust framework able to handle it. In addition, this framework may be successfully used in other applications which result in a same type of workflow.

## 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).

The target of this activity is the Bioinformatic scientific community, and in particular, those members who use a tool called "CD-HIT" which performs protein clustering on a protein sequence database. This consists in removing redundant sequences at a given sequence similarity level and generating a new database with the representatives only. This activity was proposed by CNIO (Spanish National Cancer Research Centre) and started in the context of the BioGridNet Program (www.biogridnet.org).

## 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.

For porting this application onto the Grid, we used the GridWay Metascheduler (http://www.gridway.org/) and relied on the execution services offered by BIOMED VO. GridWay is being used as a Resource Broker because its workflow management capabilities and interoperability have been proved to be very valuable. On the other hand, we are working with its Open Grid Forum (http://www.ogf.org/) DRMAA Standard (http://drmaa.org/) implementation (both C and JAVA bindings). Finally, GridWay has also been chosen because it allows interoperability with EGEE and GRIDIMadrid (http://www.gridimadrid.org/), which is a Globus-based regional testbed.

## 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 plan to start with production input data proposed by CNIO. In particular, with the analysis of various meta-genomes, starting with the first published one from Sargasso Sea.

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