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The LIBI Project: a Virtual Laboratory for Bioinformatics

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Describe the activity, tool or service using or enhancing the EGEE infrastructure or results. A high-level description is needed here (Neither a detailed specialist report nor a list of references is required).

The LIBI project (International Laboratory of BioInformatics) aims at setting up an advanced Bioinformatics and Computational Biology Laboratory. In this project a Grid Problem Solving Environment has been developed. It is based on several services such as a data federation system and a grid data access service for accessing it, a workflow management system allowing the submission on different grid middleware (gLite, Globus, Unicore) and several high throughput and high performance applications.

Report on the impact of the activity, tool or service. This should include a description of how grid technology enabled or enhanced the result, or how you have enabled or enhanced the infrastructure for other users.

The LIBI grid PSE includes a client library for the WMProxy service for submitting jobs to gLite avoiding the need of the User Interface. This library retrieves the job status by using the Logging and Bookkeeping service. Additional libraries have been implemented for the submission to the Unicore and Globus grid middleware. End-users, by using the LIBI grid portal, will be able to discovery and compose several biological applications, like as they were in a virtual laboratory. Moreover, the development of a plugin for GRelC DAS has allowed accessing the LIBI Federated DB, providing end-users and applications with search capabilities for specific biological data retrieval.

By exploiting the enhancement introduced in GridIce, a LIBI user can monitor the status of the computing resources available to the LIBI VO on the gLite grid and the execution of his jobs in order to minimize the application execution time.

Describe the added value of the grid for your activity, or the value your tool or service adds for other grid users. This should include the scale of the activity and of the potential user community, and the relevance for other scientific or business applications.

The LIBI PSE includes: i) a Grid monitoring tool, based on GridIce, for the High Throughput applications running on the EGEE infrastructure, in order to automatically recognize the user role (Site manager, VO manager, simple user) and present him the relevant information; ii) a workflow management system that allows accessing shared tools in the form of simple or composed services and their optimization. The workflow engine, based on the GRB technology, allows sharing resources belonging to gLite, Unicore and Globus; iii) an enhanced data federation database consisting of distributed biological databases, based on the Websphere Federator Server and DB2. The access in grid to the LIBI Federated DB is carried out through the GRelC Data

Access Service; iv) the porting on the grid of several relevant biological applications for studying the Bayesian inference of phylogeny, protein tertiary structure prediction etc; v) a grid portal acting as a point of access to the grid PSE.

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