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# BIOINFOGRID: Bioinformatics Grid Application for life science

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Project descriptions

The European Commission promotes the Bioinformatics Grid Application for life science (BIOINFOGRID) project. The BIOINFOGRID project web site will be available at http://www.itb.cnr.it/bioinfogrid.

The project aims to connect many European computer centres in order to carry out Bioinformatics research and to develop new applications in the sector using a network of services based on futuristic Grid networking technology that represents the natural evolution of the Web.

More specifically the BIOINFOGRID project will make research in the fields of Genomics, Proteomics, Transcriptomics and applications in Molecular Dynamics much easier, reducing data calculation times thanks to the distribution of the calculation at any one time on thousands of computers across Europe and the world.

Furthermore it will provide the possibility of accessing many different databases and hundreds of applications belonging to thousands of European users by exploiting the potential of the Grid infrastructure created with the EGEE European project and coordinated by CERN in Geneva.

The BIOINFOGRID project foresees an investment of over one million euros funded through the European Commission's "Research Infrastructures"budget.
Grid networking promises to be a very important step forward in the Information Technology field. Grid technology will make a global network made up of hundreds of thousands of interconnected computers possible, allowing the shared use of calculating power, data storage and structured compression of data. This goes beyond the simple communication between computers and aims instead to transform the global network of computers into a vast joint computational resource.

Grid technology is a very important step forward from the Web, that simply allows the sharing of information over the internet. The massive potential of Grid technology will be indispensable when dealing with both the complexity of models and the enormous quantity of data, for example, in searching the human genome or when carry out simulations of molecular dynamics for the study of new drugs.

The grid collaborative and application aspects.

The BIOINFOGRID projects proposes to combine the Bioinformatics services and applications for molecular biology users with the Grid Infrastructure created by EGEE (6th Framework Program). In the BIOINFOGRID initiative we plan to evaluate genomics, transcriptomics, proteomics and molecular dynamics applications studies based on GRID technology.

Genomics Applications in GRID
• Analysis of the W3H task system for GRID.
• GRID analysis of cDNA data.

• GRID analysis of the NCBI and Ensembl databases.
• GRID analysis of rule-based multiple alignments.
Proteomics Applications in GRID
• Pipeline analysis for domain search for protein functional domain analysis.
• Surface proteins analysis in GRID platform.
Transcriptomics and Phylogenetics Applications in GRID
• Data analysis specific for microarray and allow the GRID user to store and search this information, with direct access to the data files stored on Data Storage element on GRID servers.
• To validate an infrastructure to perform Application of Phylogenetic based on execution application of Phylogenetic methods estimates trees.
Database and Functional Genomics Applications
• To offer the possibility to manage and access biological database by using the GRID EGEE.
• To cluster gene products by their functionality as an alternative to the normally used comparison by sequence similarity.
Molecular Dynamics Applications
• To improve the scalability of Molecular Dynamics simulations.
• To perform simulation folding and aggregation of peptides and small proteins, to investigate structural properties of proteins and protein-DNA complexes and to study the effect of mutations in proteins of biomedical interest.
• To perform a challenge of the Wide In Silico Docking On Malaria.

EGEE and EGEEII future plan

BIOINFOGRID will evaluate the Grid usability in wide variety of applications, the aim to build a strong and unite BIONFOGRID Community and explore and exploit common solutions.
The BIOINFOGRID collaboration will be able to establish a very large user group in Bioinformatics in EUROPE. This cooperation will be able to promote the Bioinformatics and GRID applications in EGEE and EGEEII. The aim of the BIOINFOGRID project is to bridge the gap, letting people from the bioinformatics and life science be aware of the power of Grid computing just trying to use it. We intend to pursue this goal by using a number of key bioinformatics applications and getting them run onto the European Grid Infrastructure.
The most natural and important spin off of the BIOINFOGRID project will then be a strong dissemination action within the user's communities and across them. In fact, from one side application's experts will meet Grid experts and will learn how to re-engineer and adapt their applications to "run on the Grid"and, from the other side (and at the same time), application's experts will meet other-applications'experts with a high probability that ones'expertises can be exploited as others'solutions.
The BIOINFOGRID project will provide the EGEEII with very useful inputs and feedbacks on the goodness and efficiency of the structure deployed and on the usefulness and effectiveness of the Grid services made available at the continental scale. In fact, having several bioinformatics scientific applications using these Grid services is a key moment to stress the generality of the services themselves.

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