



## Project Presentation

### Contract Number

026808

### Project acronym

BioinfoGRID

### Project name

Bioinformatics Grid Application for life science

### Priority: Strategic Objectives

#### 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.

### Coordination of technical aspects and relation with Grid Infrastructure Projects, user training, application support and resources integration.

- To expand the Grid awareness inside the bioinformatics community.
- To identify and promote common components and solutions for the feasibility studies of the applications included in the project. Evaluate the services provided by the European Grid Infrastructure on the basis of the collection of requirements from the application WP's.
- To establish relations with Grid infrastructure projects, in particular with EGEE, to provide feedback in order to improve the European Grid Infrastructure.
- To provide the technical support required by the user and the applications WP's.

#### Dissemination and Outreach.

- To disseminate the project results to other institutions and project initiatives.
- To organize an international conference on bioinformatics.

### Participants

the following institutions will contribute to the BioinfoGRID project:

- Consiglio Nazionale delle Ricerche, Roma, Italy, represented by the Institute of Biomedical Technologies CNR-ITB Segrate (Milan), Italy acting as coordinator of the consortium
- Istituto Nazionale di Fisica Nucleare, Frascati (Roma), Italy
- Deutsches Krebsforschungszentrum, Heidelberg, Germany
- Centre National De La Recherche Scientifique, Paris, France
- The Chancellor, Masters and Scholars of the University of Cambridge, Cambridge, United Kingdom
- Consorzio Interuniversitario Lombardo per L'elaborazione Automatica, Segrate (Milan), Italy
- Steinbeis Gmbh and Co Fuer Technologietransfer, Stuttgart, Germany

### Total cost of the project

1 054 208 Euros

### Commission Funding

1 050 000 Euros

## Main goals of Specific Support Action

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.

## Key issues

The BioinfoGRID project 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 SSA will establish a common ground for collaboration between the European Grid Infrastructure providers and the Bioinformatics research user community in various fields of Bioinformatics applications (Biology, Computational Chemistry, Medicine and Biotechnology). This will be achieved through specific studies for each reference application in the Bioinformatics domain in which experts of various disciplines can collaborate on the solution of highly complex problems.

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.

## Technical approach

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.

## Expected achievements/impact

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 BioinfoGRID programme will cover the most contemporary uncharted fields of investigation in biological and medical research. The project will support studies on applications for distributed laboratory management systems for microarray technology, for gene expression studies, for gene data mining, for analysis of cDNA data, for Phylogenetics analysis, for distributed database access, for protein functional analysis and for molecular dynamics simulations in GRID. A new challenge of the Wide In Silico Docking on Malaria and an international conference for GRID Bioinformatics applications will be organized by the BioinfoGRID project.

## Coordinator contact details

Luciano Milanese  
Institute of Biomedical Technologies CNR-ITB,  
Via Fratelli Cervi 93, Segrate (Milan), 20090, Italy

## Website

For more information please visit the BioinfoGRID website:

<http://www.itb.cnr.it/bioinfoGRID>

## E-mail

Contact us at:  
[bioinfoGRID@itb.cnr.it](mailto:bioinfoGRID@itb.cnr.it)



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