

# BioGRID - An European grid for molecular biology

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Recent advances in computer technology, especially grid tools makes them good candidate for development of user interfaces to computing programs and resources. Computational grids enable sharing a wide variety of geographically distributed resources and allow selection and aggregation of distributed resources across multiple organizations for solving large scale computational and data intensive problems in science. User point of view is most important principle in the development of the UNICORE [3] software which was used to establish European computational grid - EUROGRID [2]. BioGRID is application oriented grid which adopts EUROGRID infrastructure to the specific area, namely molecular biology and quantum chemistry [1].

UNICORE is uniform interface to the computer resources which allows user to prepare, submit and control application specific jobs and file transfers. Compare to the other tools BioGRID, using UNICORE as main grid tool, has wider functionality, is more flexible and allows for much easier integration of the User interface with external quantum chemistry or biomolecular applications. Within the UNICORE environment user has a comfortable way to use distributed computing resources without having to learn for site or system specifics. Details of the UNICORE can be found elsewhere [3].

The UNICORE architecture is based, as other grid middleware, on the three tier model. It consists of user, server and target system tier. The user tier consists of the graphical user interface - UNICORE client - written as Java application.

User can specify target system and resources required for jobs using standard UNICORE client facilities. User can check job status, monitor execution and retrieve output to the local workstation. All these functions can be performed from the UNICORE client with the single login during client startup. User can monitor job status and retrieve output to any computer connected to the network with the UNICORE client installed.

We have used UNICORE as framework for development dedicated user interface to the biomolecular applications. Written in Java plugin is loaded to the UNICORE client during start, or on request. Once it is available in the client, in addition to the standard futures such as preparation of the script job, user gets access to the menu which allows for preparation application specific job. Currently plugin's are available for most popular quantum mechanical and molecular dynamics codes: Gaussian98 and Amber.

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## References

- [1] Biogrid. <http://biogrid.icm.edu.pl>.
- [2] Eurogrid. <http://www.eurogrid.org>.
- [3] Unicore. <http://www.unicore.org>.