egee

**Enabling Grids
for E-sciencE**

GRID-infrastructure in cell modeling

Tuesday 23 September 2008 16:59 (1 minute)

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 purpose of the Mathematical Cell Project (http://www.mathcell.ru) is to create the integrated mathematical model of eukaryotic cell based on GRID and distributed bioinformatics' resources. This model will help to solve some scientific and practical problems, such as novel drug design (prediction of their direct and mediated influence on cell), or the development of nanostructures and nanomaterials.

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 Mathcell Project was developed to provide the scientific community with powerful resources for calculation of extremely complicated models. It gives a novel functionality to different GRID services, creating a specific user interface that makes invisible to user all grid computing specifities. The MathCell environment is under development at the Institute of Mathematical Problems of Biology RAS. At the present it includes 3D interactive living cell model, encyclopedia of common ground notions necessary to mathematicians and biologists that are given to mathematical modeling of cell and software tools. The software is designed as a service pack to allow remote calculations in EGEE infrastructure of some interesting mathematical models of cell processes to an inexperienced grid users.

Within the limits of the Project the interactive environment was developed, which allows to perform calculations of mathematical models of basic processes in living cell using GRID infrastructure.

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Abstracts for online demonstrations must provide a summary of the demo content. Places for demos are limited and this summary will be used as part of the selection procedure. Please include the visual impact of the demo and highlight any specific requirements (e.g. network connection). In general, a successful demo is expected to have some supporting material (poster) and be capable of running on a single screen or projector.

The demo will interactively demonstrate the actual state of the Mathcell environment components and the functioning of the remote user interface of Mathcell software subsystem. The 3D interactive living cell model demonstration will be included in the demo.

The network connection will be needed.

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.

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At the present three calculable models are deployed in GRID infrastructure:
- software for mathematical modeling of electron transfer in DNA molecule;
- simulation model of electron transfer on inner photosynthetic membrane in chloroplasts;
- software for calculation of dissolution energy of biomolecules in water by MonteCarlo method.

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Track Classification: Poster