Contribution ID: **45**   Type: **Poster**

Mathcell.Ru: Integrated Mathematical Model of Living Cell in GRID infrastructure

Describe the scientific/technical community and the scientific/technical activity using (planning to use) the EGEE infrastructure. A high-level description is needed (neither a detailed specialist report nor a list of references).

Mathematical modeling of a living cell is a great challenge for modern science. Such modeling will allow ones to solve a number of practical problems, for example, acceleration of development of novel drugs and of prediction of their direct and mediated action, development of thin biochemical agents which will influence on metabolic reactions in the organism. Besides such model will be useful for development various nanostructures and nanomaterials.

Report on the experience (or the proposed activity). It would be very important to mention key services which are essential for the success of your activity on the EGEE infrastructure.

The MathCell portal includes interactive 3D cell model, encyclopedia on mathematical modeling of cell and software for modeling of some basic processes in living cell. Within the limits of the Project the interactive environment was developed, which allows to perform calculations of mathematical models in GRID infrastructure. The special Job Maintenance System was developed which automatically allows User Logging and Accounting, Job Submission, Job Status Monitoring, Job Queuing, Results Obtaining. At the present three 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 Monte Carlo method.

Describe the added value of the Grid for the scientific/technical activity you (plan to) do on the Grid. This should include the scale of the activity and of the potential user community and the relevance for other scientific or business applications

The creation of integrated mathematical model of eukaryotic cell was the aim of the Mathematical Cell (MathCell) project (http://www.mathcell.ru) realized in the Institute of Mathematical Problems of Biology RAS during the EGEE Projects. Further development of the MathCell project is closely associated with advance of Grid infrastructure, it implies integration of individual components of the model into a program system which would simulate cell processes at different levels –from microscopic to macroscopic scales and from picoseconds to the cell lifetimes.

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