

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

*Tuesday, February 12, 2008 4:00 PM (0 minutes)*

The MathCell Project includes 3D interactive living cell model, encyclopedia on mathematical modeling of cell and software for modeling of basic processes in living cell. Within the limits of the Project the interactive environment was developed, which allows to perform calculations of mathematical models using GRID infrastructure. The special Job Maintenance System was developed which automatically allows User Logging & 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.

## **If demonstration is requested please explain what visual or interactive aspects of the contribution necessitate a demonstration rather than a presentation or poster?**

The demonstration is requested because of both visual and interactive aspects. The Mathcell includes 3D interactive model of living cell, Web-interface to bioinformatics' resources, parameters setting in model interface and job maintenance in GRID.

The demonstration needs the network connection, projector and screen.

### **3. Impact**

The Mathcell Project was developed to provide biologists with powerful resources for calculation of extremely complicated models. It gives a novel functionality to different GRID services, creating a specific interface for users from computational biology.

### **URL for further information:**

<http://www.mathcell.ru>

### **4. Conclusions / Future plans**

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.

## **Provide a set of generic keywords that define your contribution (e.g. Data Management, Workflows, High Energy Physics)**

Computational Biology, Mathematical Modeling, Bioinformatics

### **1. Short overview**

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.

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**Session Classification:** Demonstrations

**Track Classification:** Existing or Prospective Grid Services