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## Construction of a Mathematical Model of a Cell as a Challenge for Science in the 21 Century and EGEE project

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As recently as a few years ago a possibility of constructing a mathematical model of a life seemed absolutely fantastic. However, at the beginning of 21-th century several research teams announced creation of a minimum model of life. To be more specific, not life in general, but an elementary brick of life, that is a living cell. The most well-known of them are: USA Virtual Cell Project (V-Cell), NIH (<http://www.nrcam.uchc.edu/vcellR3/login/login.jsp>); Japanese E-cell project (<http://ecell.sourceforge.net/>); Dutch project ViC (Virtual Cell) (<http://www.bio.vu.nl/hwconf/Silicon/index.html>).

The above projects deal mainly with kinetics of cell processes. New approaches to modeling imply development of imitation models to simulate functioning of cell mechanisms and devising of software to simulate a complex of interrelated and interdependent processes (such as gene networks). With the emergence of an opportunity to use GRID infrastructure for solving such problems new and bright prospects have opened up.

To develop an integrated model of more complex object than prokaryotic cell such as eukaryotic cell is the aim of the Mathematical Cell project (<http://www.mathcell.ru>) realized at the Joint Center for Computational Biology and Bioinformatics ([www.jcibi.ru](http://www.jcibi.ru)) of the IMPB RAS. Functioning of a cell is simulated based on the belief that the cell life is mainly determined by the processes of charge transfer in all its constituent elements.

Since (like in physics where the universe is thought to have arisen as a result of a Big Bang) life originated from a DNA molecule, modeling should be started from the DNA. The MathCell model repository includes software to calculate charge transfer in an arbitrary nucleotide sequence of a DNA molecule. A sequence to be analyzed may be specified by a user or taken from databanks presented at the site of the Joint Center for Computational Biology and Bioinformatics (<http://www.jcibi.ru>).

Presently, the MathCell site demonstrates a simplest model of charge transfer. In the framework of the GRID EGEE project any user registered and certified in EGEE infrastructure can use both the program and the computational resources offered by EGEE.

In the near future IMPB RAS is planning to deploy in EGEE a software tool to calculate a charge transfer on inner membranes of some compartments of eukaryotic cells (mitochondria and chloroplasts) through direct simulation of charge transfer with regard to the detailed structure of biomembranes containing various molecular complexes. Next on the agenda is a software tool to calculate metabolic reaction pathways in compartments of a cell as well as the dynamics of gene networks. Further development of the MathCell project implies integration of individual components of the model into an integrated program system which would enable modeling of cell processes at all levels –from microscopic to macroscopic scales and from picoseconds to the scales comparable with the cell lifetime. Such modeling

will naturally require combining of computational and commutation resources provided by EGEE project and their merging into an integrated computational medium.

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