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

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EGEE User Forum

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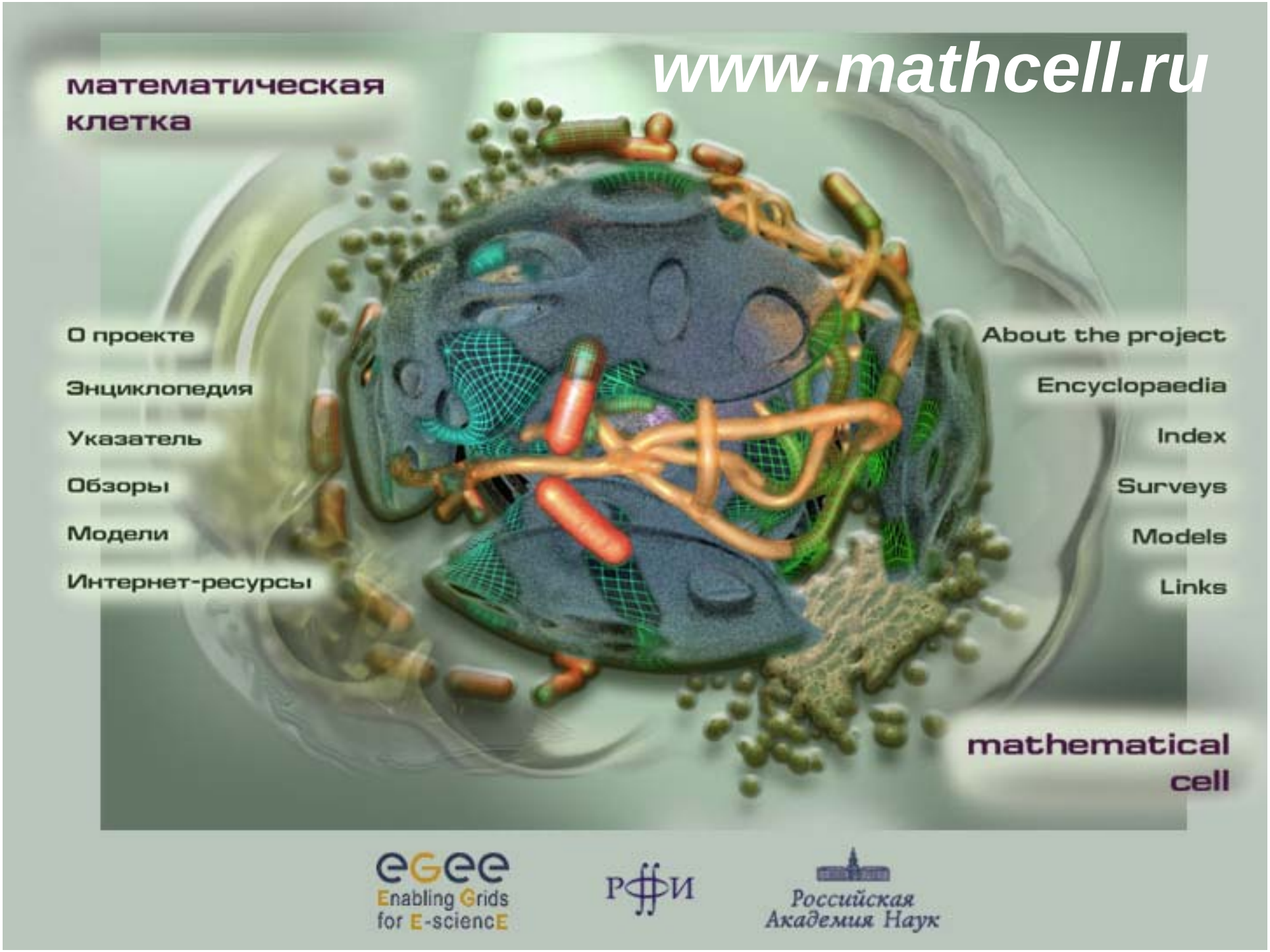
www.mathcell.ru
математическая
клетка
О проекте
Энциклопедия
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Enabling Grids
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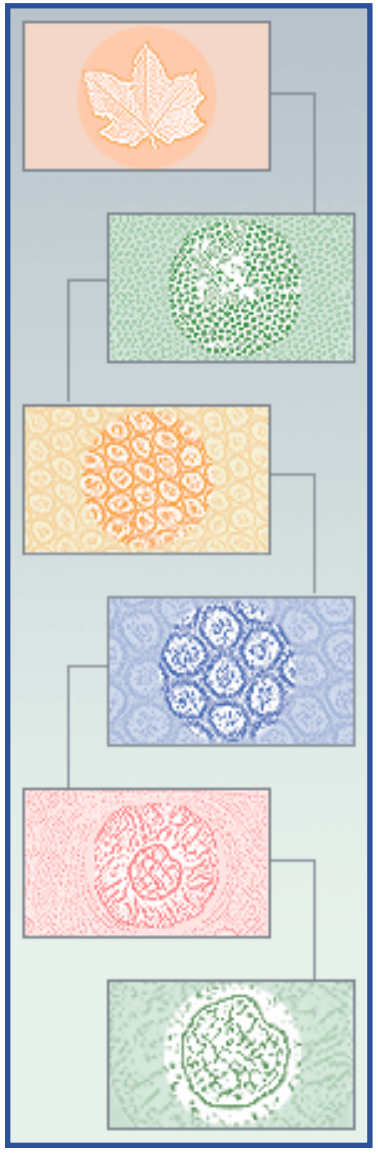
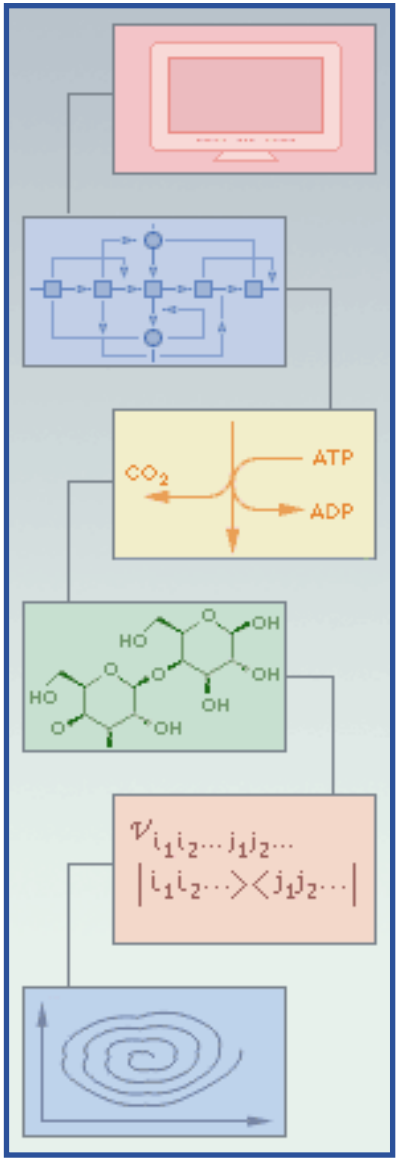
About the project



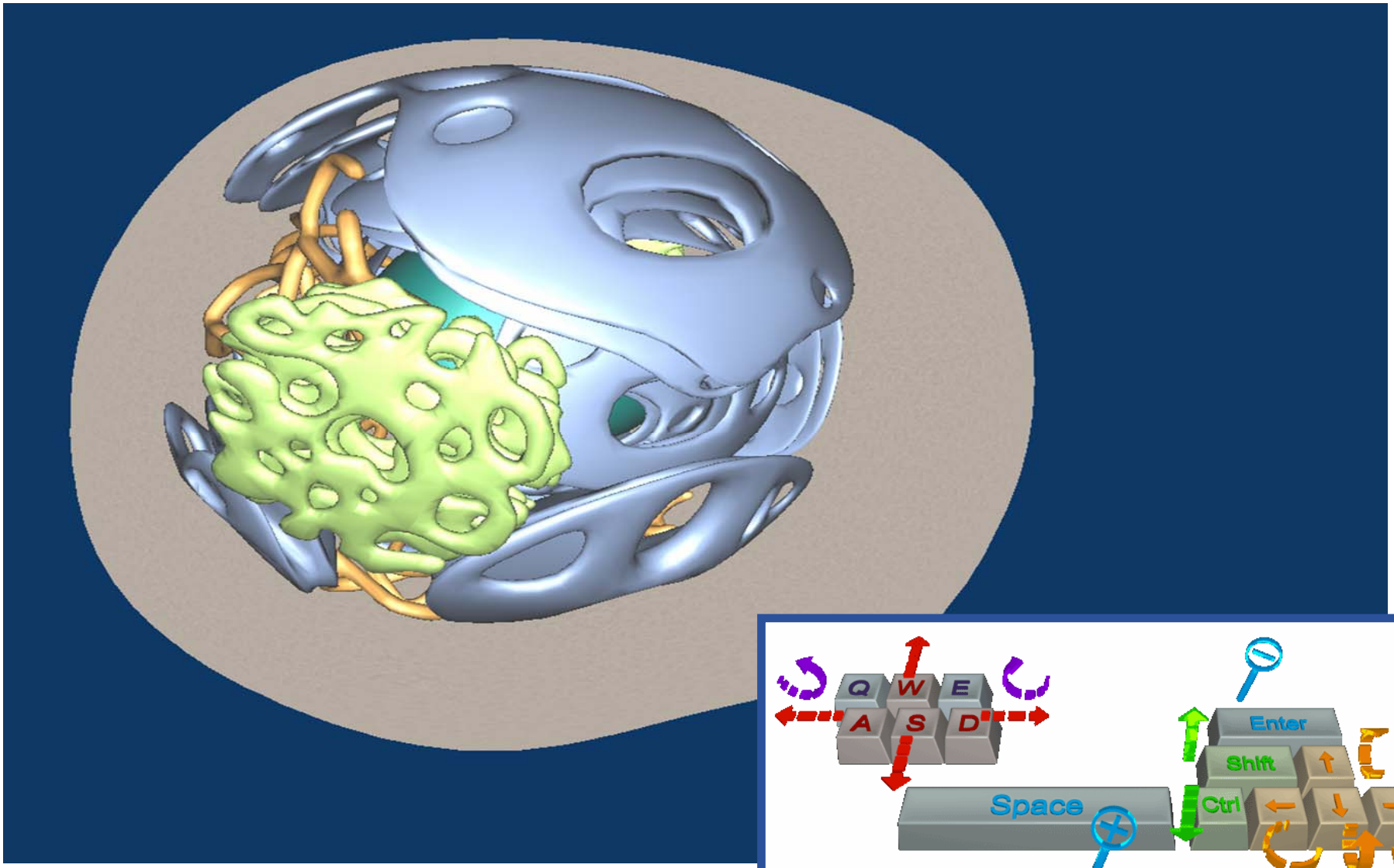
The project "MATHEMATICAL CELL" is directed on creation of the multipurpose environment for studies in biology of a living cell by integration of mathematical models, resources in bioinformatics, and computational facilities.

It will help to produce a new knowledge about a living cell, as self-consistent dynamic system.

The project is carried out by the Institute of Mathematical Problems of Biology in frames of the EGEE project. It leads to the gradual deployment of new applications in computational biology on EGEE infrastructure.



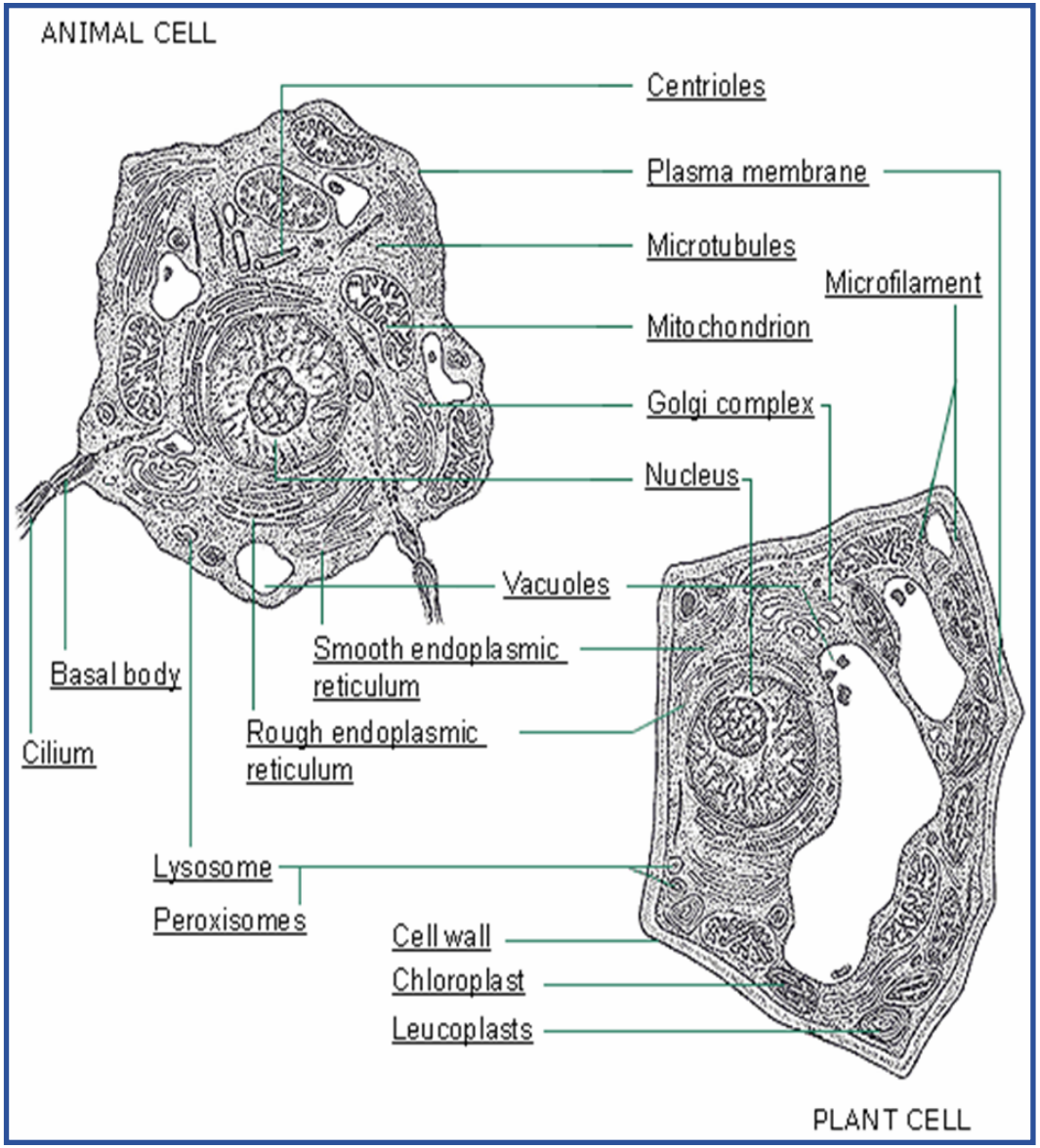
3D model of the cell



Encyclopedia

physical and mathematical knowledge

- Absolute temperature
- Bohr radius
- Chemiosmotic
- Dipole
- Electric permittivity
- Fluorescence
- Gradient
- Hamiltonian
- Interaction
- Laplacian
- Model
  - facilitated diffusion ~
  - passive diffusion transport ~
  - fluid-mosaic membrane ~
  - electron transfer ~
    - stochastic ~
    - quantum-classical ~
    - quantum-mechanical ~
    - tunneling mechanism
  - excitation transfer ~
    - inductive resonance ~
    - exchange resonance ~
    - exciton ~
  - Multiplicity
- Nonelectrolytes
- Oscillator
- Phonon
- Singlets
- Theory
- Variable
- Wave function



biological knowledge

- Acid
- Basal body
- Catabolism
- Dehydrogenization
- Electrolyte
- Fermentation
- Gene
- Histones
- Immune response
- Junction
- Krebs cycle
- Leucocyte
- Macromolecule
- NAD
  - Nitrogen base
  - Nuclear pores
  - Nucleoplasm
  - Nucleoprotein
  - Nucleotides
  - Nucleous
  - Nucleus
  - Number
    - haploid ~
    - diploid ~
- Ontogenesis
- Particles
- Reduction
- Sequence
- Telomers
- Vacuole

Links

JOURNALS

- American Journal of Physiology-Cell Physiology
- American Journal of Respiratory Cell and Molecular Biology
- Annual Review of Cell and Developmental Biology
- Biochimica et Biophysica Acta/Molecular Cell Research
- Biology of the Cell
- Cancer Cell
- Cell
- Cell & Tissue Research
- Cell Biochemistry and Function
- Cell Biology and Toxicology
- Cell Biology International
- Cell Calcium
- Cell Death and Differentiation
- Cell Growth & Differentiation

SITES

- The WWW Virtual Library of Cell Bilogy
- MIT Biology Hypertextbook Cell Biology Chapter Directory
- Клетка, толковый словарь по цитологии
- Online Biology Book
- Cell Physiology
- Cell Biology topics
- Kimball's Biology Pages
- The Silicon Cell: computing the living cell
- Silicon Cell: Mathematical/Computational Challenges
- JWS Online Cellular Systems Modelling
- National Resource for Cell Analysis and Modeling
- WWW IC Virtual Cell Development Site
- E-Cell
- SiC: The Silicon Cells

Library of mathematical models

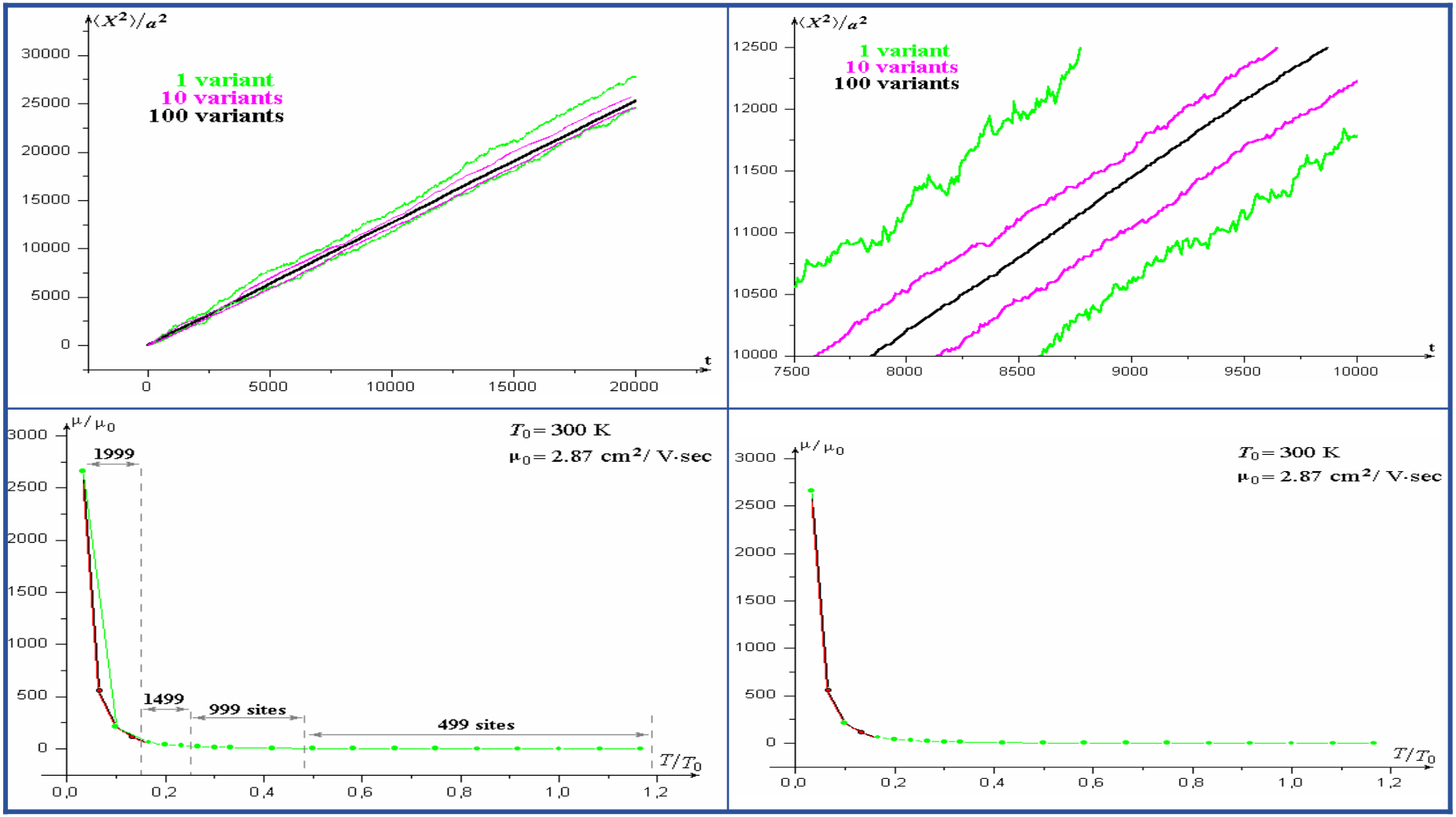
SBML LIBRARY MODELS

- Models for the Open Pathway/Genome Databases
- Minimal Mitotic Oscillator
- Minimal Mitotic Oscillator, Separate Active & Inactive Species
- Cell Cycle Model - 6 variables
- Cell Cycle Model - 2 variables
- Cell Cycle Model, 13 variables
- Minimal Mitotic Oscillator with Inhibitor
- Circadian Oscillator involving PER and TIM
- Interlocked Feedback Model of Drosophila Circadian Rhythm
- Minimal Model for Circadian Oscillations
- Most Important Fluxes in the MOMA Original E. coli Flux List
- The Hodgkin Huxley Squid Axon Model
- Repressilator
- Sporulation control network in Physarum polycephalum
- MAPK cascade with negative feedback>
- MAPK cascade in solution (no scaffold)
- MAPK cascade on a scaffold
- The Calvin Cycle in Photosynthesis

CELLML LIBRARY MODELS

- Signal Transduction Pathway Models
- Metabolic Pathway Models
- Cardiac Electrophysiological Models
- Calcium Dynamics Models
- Immunology Models
- Cell Cycle Models
- Simplified Electrophysiological Models
- Other Cell Type Electrophysiological Models
- Smooth and Skeletal Muscle Models
- Mechanical Models and Constitutive Laws

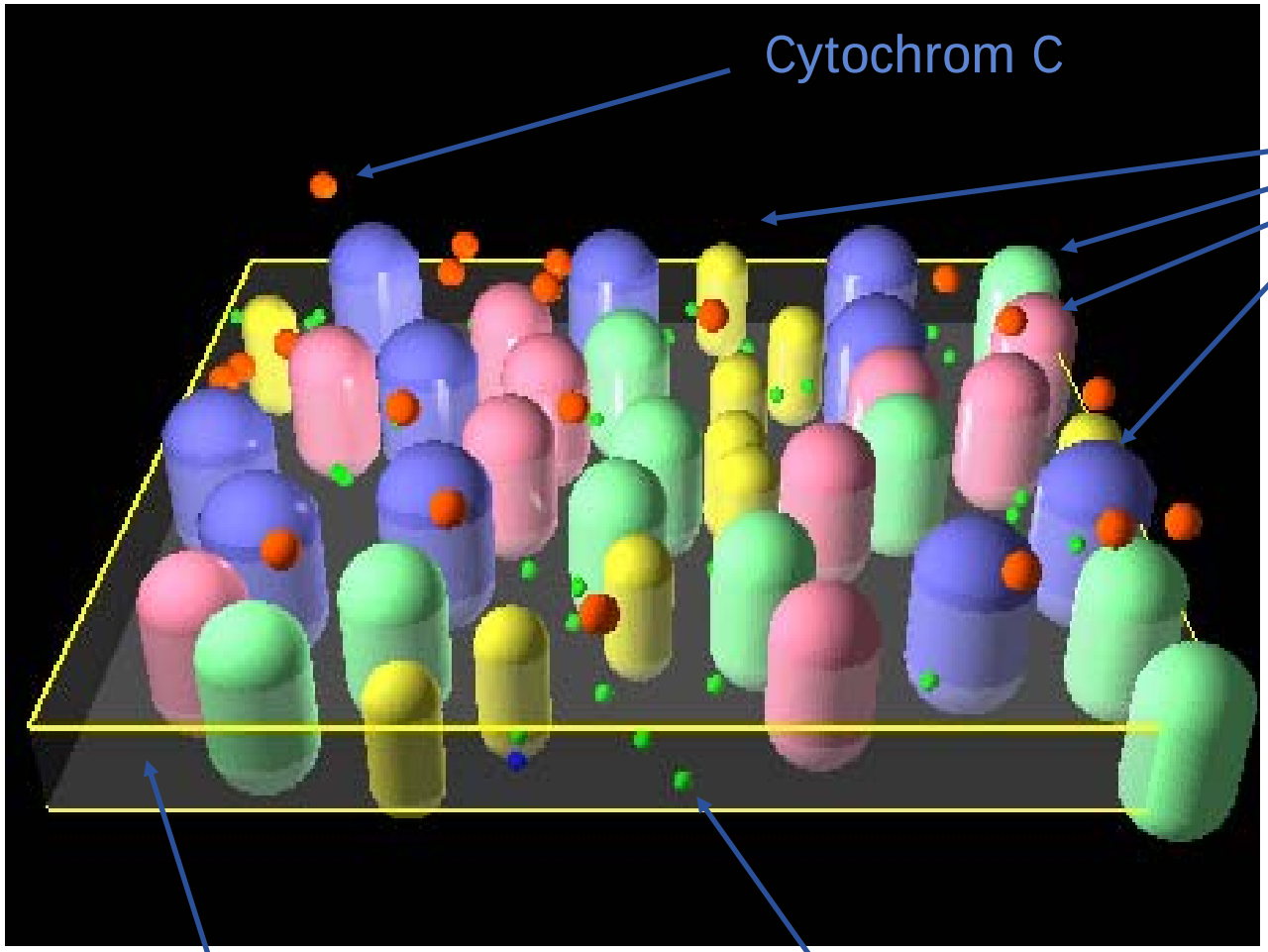
Charge transfer in DNA



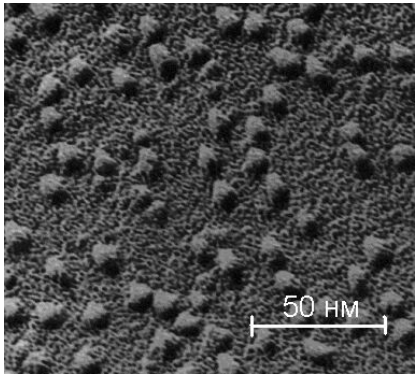
In order to estimate the average value of macroscopic physical parameters one has to calculate the large number of realizations.

Simulation models

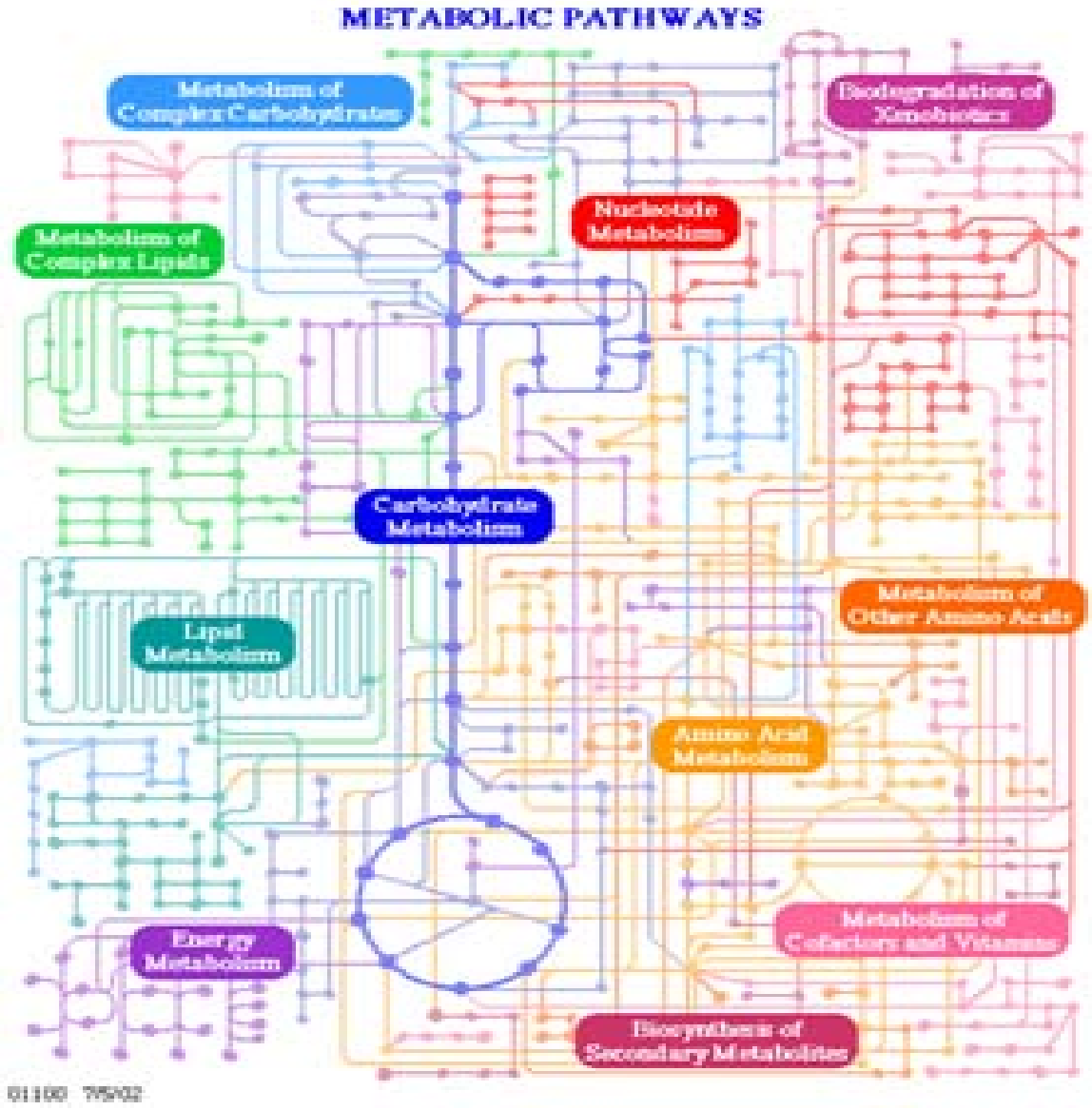
Charge transfer in mytochondrion membrane



Real mytochondrion membrane



Cellular metabolism



Mathematical modeling of cell metabolism

$$\nu_{r1}A_1 + \ldots + \nu_{rn}A_n \rightarrow \mu_{r1}A_1 + \ldots + \mu_{rn}A_n$$

$$\frac{dc_i}{dt} = \sum_{r=1}^{m} \gamma_{ri}\omega_r, i = 1,\ldots,n, r = 1,\ldots,m$$

$$\omega_r = k_r \prod_i c_i^{\nu_{ri}}$$

$$\gamma_{ri} = \mu_{ri} - \nu_{ri}$$

where

c_i - is the concentration of the i-th component of reaction,

ω_r - is the rate of the r-th reaction,

ν_{ri}, μ_{ri} - are the stoichiometrical coefficients,

γ_{ri} - is the element of the stoichiometrical matrix

Future development of MathCell

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.