The ERATO Systems Biology Workbench:
an integrated environment for multiscale & multi-theoretic simulations of molecular biology

Hamid Bolouri, Andrew Finney, Michael Hucka, Herbert Sauro,
John Doyle, Hiroaki Kitano
Caltech ERATO Kitano Systems Biology Group,
Control & Dynamical Systems, California Institute of Technology
HBolouri/AFinney/MHucka/HSauro/Doyle @cds.caltech.edu
kitano@symbio.jst.go.jp

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It is becoming increasingly clear that understanding molecular biology will require large-scale computer-based simulation and analysis of molecular interaction networks *in the context of the cell.* Interactions within cells depend not only on chemistry, but also on morphology / space, mechanical forces, the regulation of gene activity, and electrostatic and physiological factors. Appropriate software tools to allow integrated simulation and analysis of molecular systems with all of these features do not yet exist. However, several research projects are addressing the development of software tools aimed at individual aspects of molecular activity within cells. We are currently working towards the development of a software infrastructure for sharing resources and interoperability between such simulators. We refer to this multi-simulator (hence multi-theoretic and multi-scale) simulation environment as the Systems Biology Workbench. Towards this aim, we have formed an alliance of systems biology software developers whose membership includes the groups responsible for

- BioSpice (Adam Arkin et al, `http://www.lbl.gov/~aparkin/`)
- DBSolve (Igor Goryanin et al, GlaxoWellcome-SmithKlineBeecham, UK, `http://websites.ntl.com/~igor.goryanin`)
- E-Cell (Masaru Tomita et al at Keio University, Japan, `http://www.e-cell.org/`)
- Gepasi, (Pedro Mendes et al now at the Virginia Polytechnic Institute, `http://www.ncgr.org/software/gepasi/`)
- StochSim (Dennis Bray et al at the University of Cambridge, UK, `http://www.zoo.cam.ac.uk/zoostaff/morton/stochsim.htm`)
- Vcell (Les Loew et al at the University of Connecticut Health Center, `http://www.nrcam.uchc.edu/`)

Our first step has been the development of a common XML-based markup language for describing simulation data. A 24-page specification document is available at

ftp://ftp.cds.caltech.edu/pub/caltech-erato/exchange-format/