

Development of Integrated Modeling Environment for E-Cell3 System

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1 Introduction

E-Cell Project[1,2] at Keio University is aimed at the computer aided reconstruction, simulation and eventually engineering of the complete spectra of cellular phenomena. As an extension to the Ecell3 simulation environment we have developed an Integrated Modeling Environment with the 2D graphical Model Editor application as its centerpiece software. Ecell3 Model Editor is aimed at eliminating the research bottleneck at constructing, debugging and merging of large scale cell models by integrating simulation, parameter estimation, visualization tools as well as interfaces to external biological data resources such as models in SBML [3] format or biological pathway and enzyme kinetics databases..

2 Methods and Results

2.1 Design of E-Cell3 Model Editor

Model Editor is an MVC pattern two dimensional pathway editor which outputs models for or executes models in the Ecell3 Simulation environment. Command design pattern guarantees the revocability of any user action. Built in interfaces allow the export/import of data in both Ecell3 native modeling language(eml) and industry standard SBML format . The application contains a plug-in mechanism for graphically representing various biological entities, an interface to edit and compile Ecell dynamic modules, which reduces the efforts for writing and testing C++ code. Model Editor utilizes the open source Graphviz [5] visualization package to generate pathway diagrams from plain text models. The software allows merging of multiple models unifying identifiers along their E-cell3 IDs.

The application is implemented in Python language over Gtk graphical package thus portable to both Linux and Win32 platforms.

2.2 Future plans

Future plans for the Integrated Modeling Environment include support for universal model composition that would allow the merger of models from any sources by uniting models along universal annotation such as CAS or EC numbers. The modeling environment will be able to acquire pathway models from public databases and SBML model repositories. The modeling application will be able to integrate experimental time course data to compare with simulation results and perform parameter estimation using Ecell3 Session Manager. Thus Ecell3 Model Editor will be a toolbox able to perform data collection, model creation and composition, testing and debugging within the frame of one application.

2.3 Results

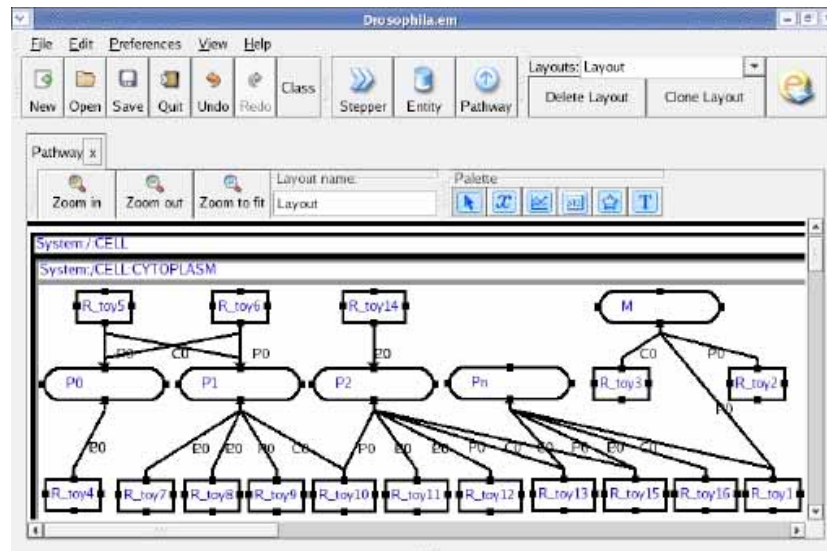


Figure 1: Screenshot of the latest version of Ecell3 Model Editor software showing automatically visualized pathway of a simple Drosophila model. .

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