

Design and development of software environment for whole cell simulation

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ABSTRACT

We have been developing E-CELL3 (E-CELL Simulation Environment Version 3.x) with the goal of establishing a technical framework for whole cell simulation. In this poster, we will describe the design and development of E-CELL3 front-ends, and the mathematical analysis methods of E-CELL3.

E-CELL 3 is being developed through reconsideration of the fundamental design and implementation methods for E-CELL 1, which was released two years ago. E-CELL3, as a whole-cell simulation platform, is designed so that development and management may continuously be carried out. E-CELL3 includes many new functions, such as compatibility in a distributed environment, modularized implementation, support of parallel computing, and description of geometric information. E-CELL3 front-ends are written in Python language, and are composed of the following three parts. Session management which manages the processes of simulation and analysis, user interfaces such as GUI and CUI, and various mathematical analysis modules.

We are also developing EML (E-CELL Model description Language), which is a language for describing cell models using E-CELL3 simulation environment. In E-CELL1, cell models were constructed using a primitive method of editing the original rule file written via a spread sheet. EML is defined as a subset language of XML. It is able to perform advanced processing, such as error check of a model and compatibility of the data with other MDLs (SBML, CellML and etc ...).

In order to show the validity of a cell model, a technique for mathematically verifying a model is required. Therefore, the introduction of various mathematical analysis techniques is indispensable. We have carried out forefront research on mathematical analysis techniques, such as time series analysis / metabolism control theory, and optimization techniques. These methods are implemented as a part of E-CELL 3 front-end. As a result, E-CELL 3 is not just a simulator, but is an integrated software environment for construction and analysis of a cell model.

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