Designing Object-based Cell Simulation System: E-CELL 3

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ABSTRACT

We have been developing a software environment for whole cell scale modeling, simulation and analysis since 1996[1] for E-CELL Project[2]. E-CELL Project is an international research project aiming at developing necessary theoretical supports, technologies and software platforms to allow precise whole cell simulation.

After releasing version 1.0 of E-CELL Simulation Environment(Serizawa) in 2000, we have been redesigning the software for greater flexibility and advanced functionality, and are planning for release of version 3(Hekkoro) by the end of this year. Hekkoro, or E-CELL 3, is being developed for the purpose of providing the cell simulation community a common, highly flexible and high-performance software environment, which will be used as the community standard platform for at least 10-15 years. In this poster, we will describe an overview of the ongoing E-CELL3 development project, putting an emphasis on the system architecture and simulation engine.

The basic architecture, or the core simulation software of E-CELL 3, is a set of extension modules for Python language interpreter, written in C++/C/Python. This consists of a libecs cell modeling toolkit, an E-CELL Micro Core(EMC) layer, a python language binding(PyECS), and other peripheral python modules. Libecs, code-named Koyurugi, is a generic object-oriented C++ class library for constructing various object-based cell models. One of the distinct features of Koyurugi is that the constructed cell models themselves work as simulation engines. E-CELL Micro Core(EMC) defines interfaces and implementations of Simulator class, which provides a simple API of the Koyurugi class library. PyECS is a Python binding of the EMC. It can be viewed as an adapter for the EMC to make it act as an extension module of the Python language interpreter.

The simulation engine of E-CELL 3 is Koyurugi, which is a class library for cell modeling and simulation. Because there are various subsystems with diverse computational properties in a single precise cell model, no cell model, which are non-trivial, can be efficiently simulated using a single computation method. To overcome this obstacle, E-CELL3 will allow various time scales and many computation algorithms(ex. SRM object-models, ordinary/partial differential equation solvers, stochastic computations etc…) to co-exist in a single model.

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REFERENCES

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