

Development of the New Modular Simulation Engine for E-CELL Simulation Environment

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1 Introduction

Complex nature of biological systems arose from diversity of components and underlying rules, rather than emerging complexity from homogeneity and a few principles in physics and chemistry, characterize biology. This is one of the reasons why sophisticated software science is demanded in cellular simulation projects, unlike the other usual computational science fields like computational physics in which its necessity is relatively neglected. Software science can support the cellular simulation projects in many ways including: sophisticated modeling theory, well-designed software platform, data management methods, project management etc.

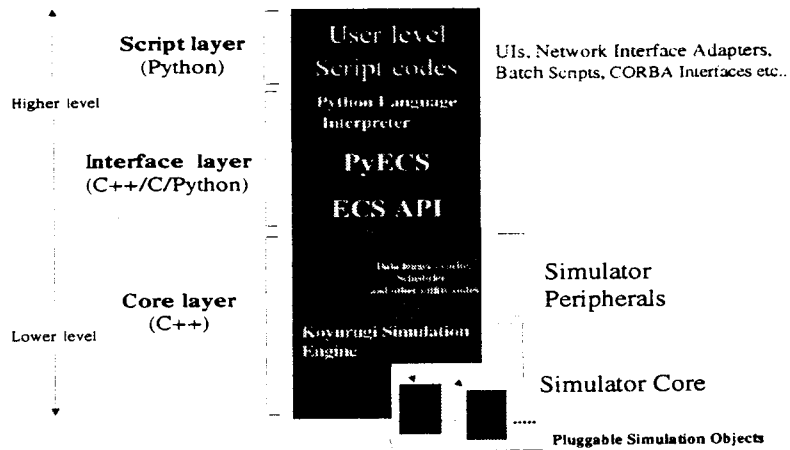
Among many efforts in E-CELL Project, we will concentrate on design and construction of the software platform in this presentation.

2 E-CELL Simulation Environment

We have been developing a software environment for whole cell scale modeling, simulation and analysis since 1996[1]. After releasing version 1.0 of E-CELL Simulation Environment (Serizawa) in early 2000, we have been attempting redesign of the software for greater flexibility and advanced functionalities (version 3).

3 Architecture

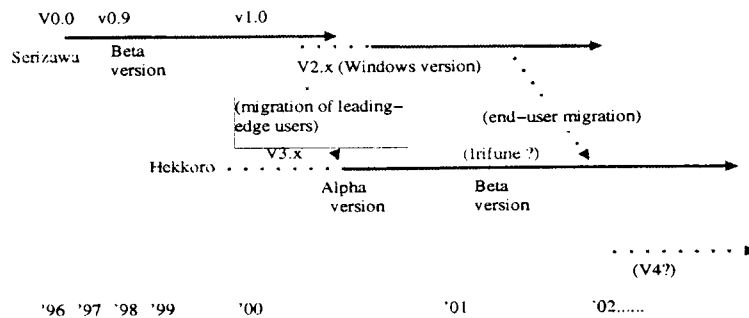
Core simulation software (E-CELL Core System) of the version 3 is Hekkoru, which is actually a set of extension modules of python language interpreter written in C++/C/python. It consists of Koyurugi simulation engine, python API (PyECS) and other peripheral modules. The API layer and the simulator core layer are designed to be isolated to each other running as separate execution threads. Any fashion of user interfaces can be constructed as user-level python scripts.



4 The Simulation Engine

Koyurugi is a generic object-oriented class library to construct various cell models. One of the distinct features of E-CELL Core System is that the constructed cell models themselves work as simulation engines. In this sense, Koyurugi can be viewed as a toolkit for constructing cell simulators. Users can define their own task-specific simulation objects which can be dynamically loaded.

In order to handle various kinds of simulation schema and wide range of time scale in a single model, users can define multiple computation units among which simulation algorithm and time step size can vary. Support for diffusion system and stochastic simulation methods as in StochSim[2] are planned to be implemented.



Acknowledgements

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References

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