

E-CELL Simulation Environment Version 3: System Architecture of Simulation Engine

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1 Introduction

E-CELL Simulation Environment, a software environment for whole-cell modeling, simulation and analysis, has been under development since 1996 [1] by the E-CELL Project [2]. The goal of E-CELL Project, an international research project, is to develop and innovate the theoretical supports, technologies, and software platforms necessary for precise whole-cell simulation.

After releasing E-CELL 1 (E-CELL Simulation Environment Version 1) two years ago, we have been redesigning the software for greater flexibility and advanced functionality, and on September 2001, we released the alpha-version (ecell-3.0a1) of E-CELL 3 (E-CELL Simulation Environment Version 3) [3]. The beta-version of E-CELL 3 is planned to be released by the end of this year.

E-CELL 3 is being developed with the purpose of providing the cell simulation community a common, highly flexible and high-performance software environment. In this poster, we will describe the system architecture and simulation engine for E-CELL 3.

2 System Architecture

The system 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), plus other peripheral python modules. Libecs, also called 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.

3 Simulation Engine

Koyurugi, the simulation engine of E-CELL 3, is a class library for cell modeling and simulation. Because there are various subsystems with diverse computational properties in a single precise cell model,

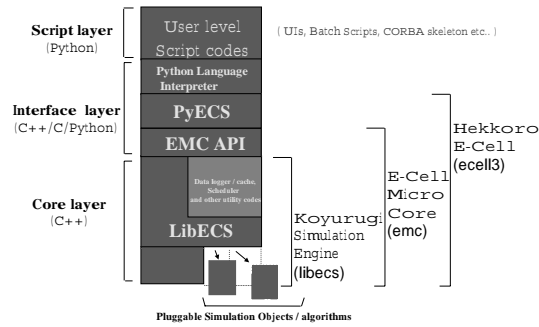


Figure 1: Three-layer architecture of E-CELL 3.

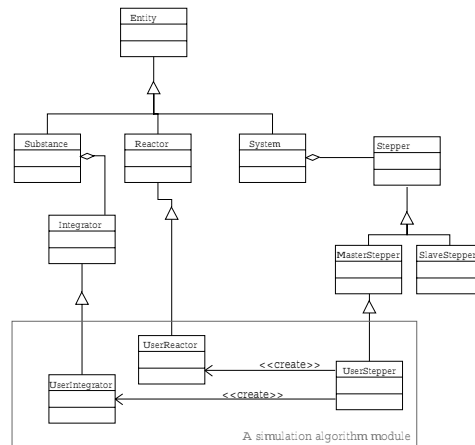


Figure 2: UML representation of a pluggable algorithm module and its related classes.

a non-trivial cell model cannot be efficiently simulated using a single computation method. To overcome this obstacle, E-CELL 3 will be implemented to allow various time scales and many computation algorithms (ex. SRM object-models, ordinary/partial differential equation solvers, stochastic computations etc.) to coexist in a single model.

Acknowledgments

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References

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- [3] http://bioinformatics.org/?group_id=46