

# Biopathway Model Conversion from E-CELL to Genomic Object Net

Mika Matsui<sup>1</sup>

mika@m.oshima-k.ac.jp

Atsushi Doi<sup>2</sup>

atsushi@ib.sci.yamaguchi-u.ac.jp

Hiroshi Matsuno<sup>2</sup>

matsuno@sci.yamaguchi-u.ac.jp

Yuichi Hirata<sup>3</sup>

hirata@ims.u-tokyo.ac.jp

Satoru Miyano<sup>3</sup>

miyano@ims.u-tokyo.ac.jp

<sup>1</sup> Department of Electronic-Mechanical Engineering, Oshima National College of Maritime Technology, 1091-1, Komatsu, Oshima-cho, Yamaguchi 742-2193, Japan

<sup>2</sup> Faculty of Science, Yamaguchi University, 1677-1, Yoshida, Yamaguchi-shi, Yamaguchi 753-8512, Japan

<sup>3</sup> Human Genome Center, Institute of Medical Science, University of Tokyo, 4-6-1 Shirokane-dai, Minato-ku, Tokyo 108-8639, Japan

**Keywords:** E-CELL, Genomic Object Net Assembler, conversion procedure

## 1 Introduction

E-CELL [3] is a conceptually attractive biosimulation tool for representing and simulating biopathways. With E-CELL, Tomita *et al.* [4] have modeled several biopathways including biochemical reactions in human erythrocyte, signal transduction for bacterial chemotaxis, energy metabolism in mitochondria and lytic-lysogenic switch network of  $\lambda$  phage.

On the other hand, we developed a tool for representing and simulating biopathways called “Genomic Object Net (GON) Assembler” which uses hybrid functional Petri net (HFPN) as a basic mechanism for representing biopathways [1] where XML documentation of biopathways and their simulations is also realized as another tool in Genomic Object Net [2].

The purpose of this paper is to show a procedure for converting biopathway models with E-CELL to the ones executable on GON Assembler. Thus E-CELL can be regarded as a subset of Genomic Object Net. A conversion program of E-CELL to GON Assembler is being developed.

## 2 Constructing HFPN from E-CELL Model

In E-CELL, a system of biopathways is represented with a spread sheet compiling substances and reactions with ordinary differential equations (ODEs), as is shown in Figure 1(a). For reactions which cannot be represented with ODEs, it employs *ad hoc* user-defined C++ programs called postern reactor. In the following, we show a rough sketch of procedure for obtaining HFPN by converting E-CELL biopathway models.

1. Assign a continuous place to each of substances in E-CELL spread sheet.
2. Describe HFPNs which correspond with E-CELL reactors.
3. Combine HFPNs obtained above at a continuous place of common substance in two (or more) E-CELL reactors.
4. Determine firing speeds of continuous transitions by referring constants described in E-CELL spread sheet.

Figure 1(b) is an example of HFPN converted from E-CELL.

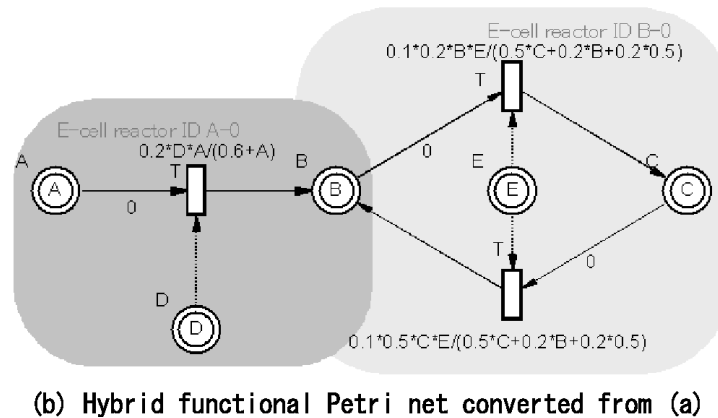
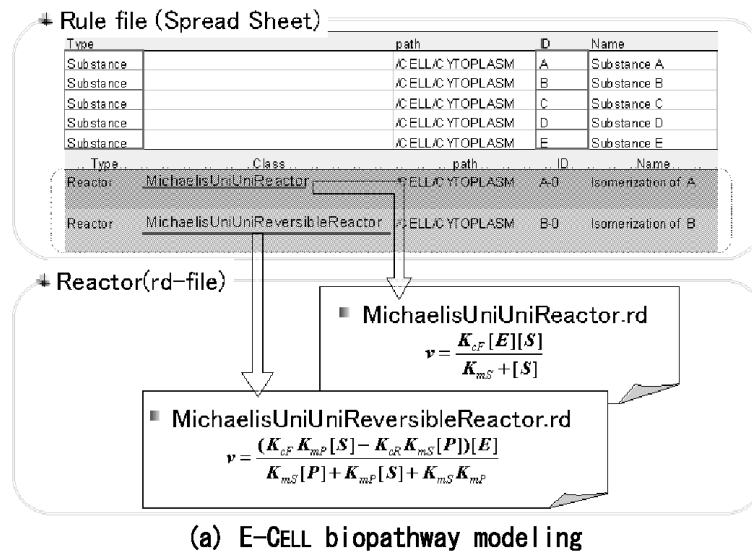


Figure 1: Conversion from E-CELL to Genomic Object Net.

## Acknowledgments

This work is partially supported by the Grand-in-Aid for Scientific Research on Priority Areas (C) “Genome Information Science” and Grand-in-Aid for Scientific Research (B) (No.12480080) from the Ministry of Education, Culture, Sports, Science and Technology in Japan

## References

- [1] Matsuno, H., Doi, A., Tanaka, Y., Aoshima, H., Hirata, Y., and Miyano, S., Genomic Object Net: Basic architecture for representing and simulating biopathways, *submitted*, 2001.
- [2] Matsuno, H., Doi, A., Hirata, Y., and Miyano, S., XML documentation of biopathways and their simulations in Genomic Object Net, *Genome Informatics*, 12, 2001.
- [3] Tomita, M. *et al.*, E-CELL:Software environment for whole cell simulation, *Bioinformatics*, 15, 72–84, 1999.
- [4] Tomita, M. *et al.*, The E-CELL project: Toward integrative simulation of cellular processes, *Proc. 4th Annual International Conference on Computational Molecular Biology*, 290–298, 2000.