Distributed Collaborative and Interactive Simulation of Large Scale Biochemical Networks

Mostafa Herajy and Monika Heiner
Brandenburg University of Technology at Cottbus
Data Structures and Software Dependability

Framework

Users

Steering Application Programming Interface

Steering GUI

Components

- Steering server
- Steering graphical user interface (GUI)
- Steering application programming interface (Steering API)
- Simulators (internal and external)

Features

- Intuitive and understandable representation of reaction networks with the help of Petri nets
- Distributed collaborative and interactive simulation of biochemical networks
- Tight coupling of visualization and simulation
- Extendibility to include further simulators provided by the users
- Support for coloured and uncoloured Petri nets

Simulators

- Deterministic (ODEs)
- Stochastic (SSA)
- Hybrid with static partitioning
- Hybrid with dynamic partitioning
- User-defined simulator

Case Study

Circadian Oscillation Model

References


Implementation

- Implemented in C++
- Platform-independent
- Implemented using wxWidgets

Outlook

- Condition-based steering
- Backtracking
- Steering the model’s structure
- Wrapper APIs
- Web-based and mobile steering GUI

Strengths

- Web-based and mobile steering GUI
- Steering the model’s structure
- Wrapper APIs
- Web-based and mobile steering GUI

Weaknesses

- Condition-based steering
- Backtracking
- Steering the model’s structure
- Wrapper APIs
- Web-based and mobile steering GUI

Steering API

Simulators (internal and external)

More accurate

Hybrid

Stochastic

Deterministic

Internal Simulator

PN definition

Model Views

Change parameters

Result output

Steering Application Programming Interface

User 1

User 2

User N

Steering Application Programming Interface

Steering

Visualization

Steering

Visualization

Steering

Visualization

Steering

Visualization

Steering Application Programming Interface

User M

Model 1

PN definition

Model Views

Change parameters

Result output

Internal Simulator

Model 2

PN definition

Model Views

Change parameters

Result output

Internal Simulator

Model N

PN definition

Model Views

Change parameters

Result output

Internal Simulator

External Simulator 1

External Simulator 2

External Simulator N

Change parameters

Result output

Internal Simulator

Steering GUI

External Simulator (optional)

Continuous Simulation Output

Circadian Oscillation Model

Graphical User Interface (Steering API)