The ERATO Systems Biology Workbench

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Introduction

The ERATO Systems Biology Workbench (SBW) is an extensible software framework enabling the creation of an integrated, easy-to-use software environment that allows the sharing of models and resources between simulation and analysis tools for systems biology. In this paper we summarize the project goals and current status.

Goals of the SBW Project

- Integrate a variety of software tools that implement different approaches to modeling, parameter analysis, and other related tasks
- Enable the construction of complex hierarchical biochemical models from arrays of model components
- Enable the interaction with biologically-oriented databases containing data, models and other relevant information

Principles of the SBW Project

- Be open-source: use a variant of the GNU library license
- Be portable: Windows and Linux
- Use current and emerging standards such as Python 2 and the Systems Biology Markup Language (SBML)
- Ensure tools are easy to use
- Reduce the time spent by developers both creating software infrastructure and creating tools that exist in a similar form in other packages, allowing developers to concentrate on the development of new algorithms and models
- Use the workbench as a vehicle for collaboration between developers of bioinformatics technology

Architecture

To facilitate modularization and extensibility, SBW is a software framework that enables separately compiled modules or plug-ins to be recombined to form a functioning application. Currently, plug-ins can either be applications, dynamic libraries or Java JAR files. Plug-ins can be created in several programming languages. SBW currently employs components written in Delphi and Java, and we have written plug-ins in C++. We plan to create bridges to other languages including Python.

Intercommunication between plugins is performed by simple message passing mechanisms. Plug-ins are registered with a directory. This directory indexes plug-ins by category. A category groups together plug-ins with a common interface.

Phase 1

This phase provides a GUI for drawing biochemical pathways. The Designer exports the model in SBML format. The SBW integration allows the user to select an analysis to be invoked on the model.

Jarnac

This phase provides the following QDE-based analyses: Time-Based simulation, Steady state analysis and Metabolic Control Analysis.

Optimization

This allows the fitting of model parameters to experimental data.

Phase 2

Bifurcation

We will integrate a standard bifurcation tool.

3D Plotting

We will integrate 3D plotting functionality to support time based simulation and bifurcation analyses.

Phase 3

Multi-scale simulation

We will develop a new time-based simulation component that will enable very fast yet accurate simulation of biochemical networks. This simulator will combine stochastic and DEE techniques using novel algorithms developed in collaboration with leading researchers in the field.

Transparent database access

We will develop a several plugins to enable the user to download models from bioinformatics databases.

Modular and Multi-cellular models

As part of phase 3 we will enable SBML Level 2 support by:

- Extending and developing model capture tools to support hierarchical models
- Developing a tool that translates SBML Level 1 from Level 2 to enable existing analyses to be applied to Level 2 models.

Packaging

We plan to create a Windows installation as part of phase 1 and a Linux installation as part of phase 2. These packages will include plug-ins as they become available and tutorials with working models supplemented later by online documentation. We plan to set up web resources appropriate to open source development, including a public bug database.

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Jarnac - http://members.tripod.co.uk/sauro/bioiact.htm