The Systems Biology Workbench (SBW) Version 1.0: Framework and Modules

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Introduction
Progress in molecular biotechnology has fueled an explosion in the development of software tools. Regrettably, developers often end up recreating similar facilities in separate software packages. In an effort to make it more attractive for developers to share rather than reinvent such tools, we have implemented the Systems Biology Workbench (SBW), a free, open-source, application integration environment. Our goal has been to create a framework simple enough that software authors find it easy to provide an SBW interface than to recreate functionality available in other tools. By doing so, we hope developers can concentrate on creating best-of-breed solutions in their areas of expertise.

What Does SBW Provide?
SBW provides libraries for enabling applications to learn about and communicate with each other. The applications may be running on separate computers.

The SBW Broker
The SBW Broker starts applications on demand, and coordinates their execution on a given computer. A Broker is started automatically for the user if one is not running when the first SBW application starts.

Features of SBW Version 1.0
• Languages supported: C, C++, Delphi, Java, Perl, Python, and R.
• Windows (98, 2000, XP) and Linux supported, with MacOS X planned in the near future.
• Secure, distributed operation via SSH, featuring remote startup of brokers and applications.
• CORBA gateway for bidirectional communication between SBW-based apps and CORBA-based apps.
• Collection of basic applications provided with the SBW distribution, including:
  • A simple stochastic simulator based on the Gibson-Bruck variant of the Gillespie algorithm
  • An SBML-to-MATLAB ODE & Simulink translator
  • An SBML reader tool that allows a program to extract (via an API) components of an SBML model
  • A “clipboard” module that stores an SBML model description, and allows the easy transfer of models between separate modules
  • A “browser” module that allows querying SBW for registered models and producing descriptions of each module’s interface in Java or CORBA IDL
  • A simple plotting module for time-series data
  • A generic simulation control GUI interface
  • A collection of tutorial example modules in C, C++, Delphi and Java
• Extensive documentation—in addition to overview documents and published papers, every language library has its own programmer’s manual and API reference.

SBW in Action: A Sample Session
Here is an example of using several SBW-enabled tools to create and simulate a two-compartment model of a hypothetical single-gene oscillatory circuit.

In this highly simplified model, there is a gene G, which encodes its own repressor, and is transcriptionally activated at a constant rate, v1. Transcriptional activation of a gene G (which normally involves many enzymatic reactions) is summarized here as the production of active RNP from source material, tRNA, and degradation to base. Transcribed mRNA is then transported from the nucleus into the cytoplasm, where it is translated to the product P from constituent amino acids AA and where it is also subject to degradation.

Model Visualization and Analysis
Setting the run parameters for the simulation and selecting the output variables in the simulation control GUI allows the user to plot the values of quantities over time. The plot at the right shows how the concentrations of AA and P in the model oscillate over time.

A user can also perform other analyses on the model via SBW, e.g., by invoking the bifurcation analysis module.

Third-Party Modules Available For SBW
• JDesigner, a biochemistry simulation package for Windows
• Posamentis Tools, a simple interactive ODE solver
• A stochastic simulator based on Gillespie’s algorithm
• A bifurcation analysis module
• An optimization module
• An SBML validator for checking SBML model EEs
• An Inspector that lists running modules & their services

Coming Attractions
More open-source developers are joining the SBW project, and together we are enhancing and extending SBW in many ways. Here is a preview of coming attractions:

• Support for JDK 1.4
• Support for MacOS X
• Bidirectional SOAP-SBW gateway
• JDesigner, a visual biochemistry network layout tool
• New modules, including:
  • Improved generic GUI for simulators
  • Improved, full-featured plot module
  • New simulation engines

How to Get Started with SBW
The SBW version 1.0 package and extensive documentation are available from the project web site, http://www.sbw-tools.org. SBW is distributed under the terms of the GNU LGPL.

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