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SBW TUTORIAL

INSTALLATION

Install from the web site sys-bio.org

The screenshot shows the website sys-bio.org in a browser window. The page features a navigation menu with links for Home, Downloads, News, Research, Papers, About Us, Contact Us, SBW Help, and Jobs. The main content area is titled "Announcing the Joint SBW & CompuCell3D Workshop August 2011" and includes a section for "Version 2.8.3 SBW July 2011". A red circle highlights the link "DOWNLOAD Windows version of Systems Biology Workbench: 2.8.3". Below this link, there is a note about installing 2.8.2 and finding the update utility. The page also features several news items, including "May 09 2011: New Version of TinkerCell", "Feb 02 2011: Fan-out in Gene Regulatory Networks", "Jan 14 2011: Nature Biotech Letter on Synthetic Biology", and "Nov 22 2010: Robust Synthetic Circuits".

University of Washington x +
sys-bio.org
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sys-bio.org
Computational Systems Biology
Sauro Lab
University of Washington

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What is SBW
Research Impact
Published Papers
Lab Members
Available Positions
CSB Links
Courses
Student Projects

Online Services:
SBML Layout Viewer
SBML Validation
SBML Simulation
SBML Translator
Web Service Creation
Model Repository

Software Downloads:
1. SBW
2. JDesigner
3. Jarnac
4. WinSCAMP
5. Matlab Interface
6. Optimization
6. Bifurcation

maintained by Frank Bergmann

SOURCEFORGE.NET

Announcing the Joint SBW & CompuCell3D Workshop August 2011
We are pleased to announce Joint User-Training Workshop "Developing Multi-Scale, Multi-Cell Developmental and Biomedical Simulations with CompuCell3D and SBW". It will focus on teaching the basics of multi-cell, multi-scale modeling using the open-source packages CompuCell3D and SBW. For more information see our Workshop Page

Version 2.8.3 SBW July 2011
We are pleased to announce the release 2.8.3 of the Systems Biology Workbench.

DOWNLOAD Windows version of Systems Biology Workbench: 2.8.3
Go to Sourceforge page for other OS specific downloads
This link will actually install 2.8.2, however find the update utility in the start menu under the Systems Biology Workbench entry and start the update, this will retrieve and install 2.8.3.

Announcement: Modeling Webinar Hosted by Rosa
A Webinar will be held on Tuesday 26th of July at 12:00 to 1:00 pm EDT on Standards and Software in Biomedical Systems Modeling. Register here if you wish to attend
The webinar will describe the development of biomedical modeling standards during the last 10 years and how that has stimulated a great many other initiatives. Dr Sauro will also describe software developments he has been involved in and possible future developments in high performance computing and real-time simulation. He will demonstrate software and discuss future plans for the current suite of systems biology modeling tools.
Rosa is a company that specializes in creating robust mathematical models that simulate drug effects and trial outcomes. See their Web site for further details.

Group Blogs and Web Pages
Visit our group blogs at:
TinkerCell Blog by Deepak Chandran
AnalogMachine Blog: Cells, Networks and Computation

May 09 2011: New Version of TinkerCell
There is a new version of TinkerCell available. The new version incorporates ruby scripting, octave scripting, callback functions from Python and Octave, optimization and global sensitivity plugin, improved display features plus numerous bug fixes (www.tinkerCell.com).

Feb 02 2011: Fan-out in Gene Regulatory Networks
In synthetic biology, gene regulatory circuits are often constructed by combining smaller circuit components. Connections between components are achieved by transcription factors acting on promoters. If the individual components behave as true modules and certain module interface conditions are satisfied, the function of the composite circuits can in principle be predicted. This paper describes how the fan-out of a genetic circuit can be defined - J Biol. Eng (2010) Kim & Sauro, 4:16.

Jan 14 2011: Nature Biotech Letter on Synthetic Biology
Joint letter to Nature Biotechnology published: Essential information for synthetic DNA sequences, volume 29(1), January 2011 Nature Biotechnology

Nov 22 2010: Robust Synthetic Circuits
New paper published: Designing and engineering evolutionary robust genetic circuits in Journal of Biological Engineering, 4:12, 2010, doi:10.1186/1754-1611-4-12. An investigation into what enables synthetic circuits to

INSTALLATION

From jdesigner.sf.net

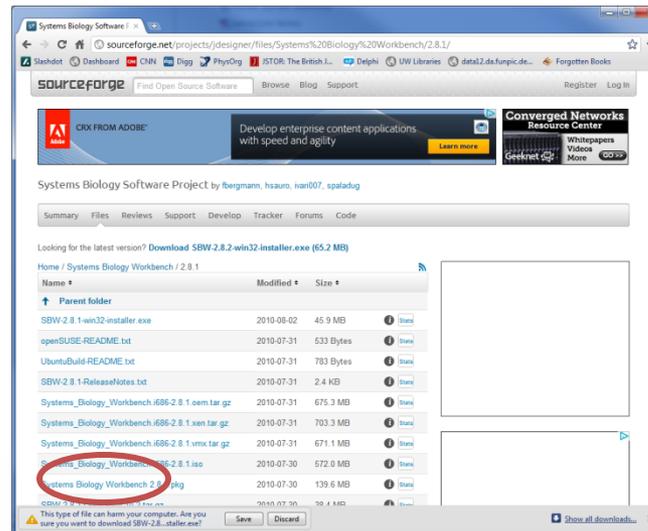
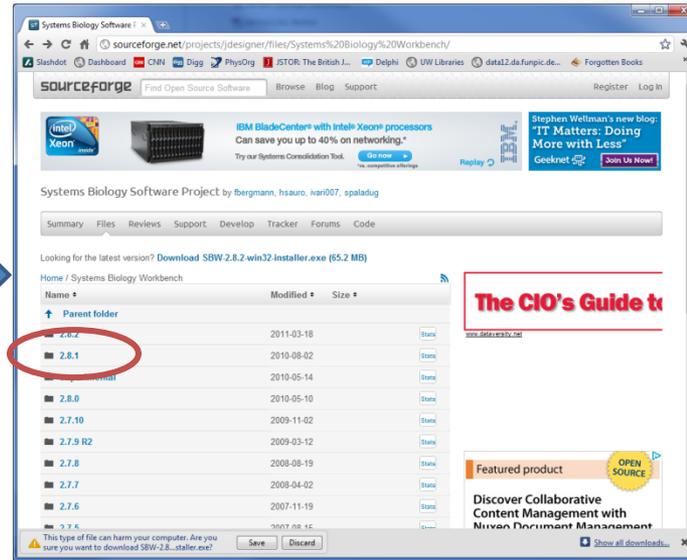
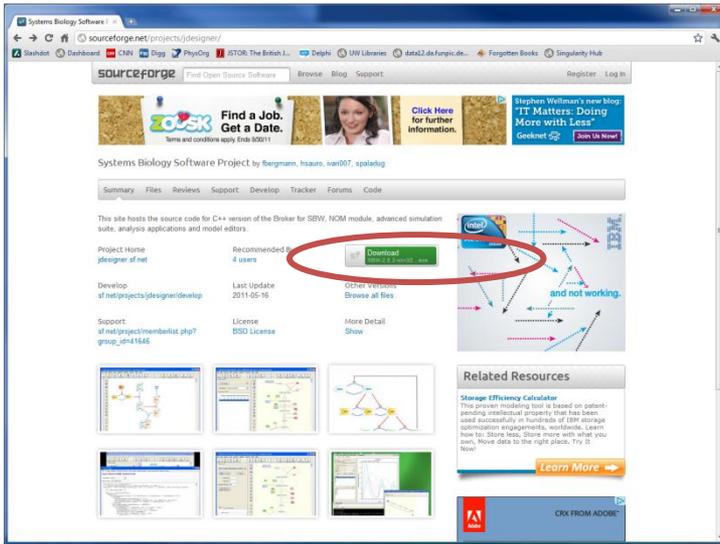
The screenshot shows a web browser window displaying the SourceForge project page for Systems Biology Software. The browser's address bar shows sourceforge.net/projects/jdesigner/. The page features a navigation bar with 'sourceforge', search, and 'Browse Blog Support' links. Below the navigation bar are several advertisements, including one for ZOOSK and another for Stephen Wellman's blog. The main content area is titled 'Systems Biology Software Project by fbergmann, hsauro, ivan007, spaladug'. It includes a summary section with tabs for 'Summary Files Reviews Support Develop Tracker Forums Code'. A description states: 'This site hosts the source code for C++ version of the Broker for SBW, NOM module, advanced simulation suite, analysis applications and model editors.' A table of project details is visible:

Project Home jdesigner.sf.net	Recommended By 4 users	Download SBW-2.9.2-win32.exe
Develop sf.net/projects/jdesigner/develop	Last Update 2011-05-16	Other Versions Browse all files
Support sf.net/project/memberlist.php?group_id=41646	License BSD License	More Detail Show

To the right of the table is a diagram with arrows and the text 'and not working.' Below the table are several screenshots of the software interface. A 'Related Resources' section features a 'Storage Efficiency Calculator' with a 'Learn More' button. At the bottom right, there is an advertisement for 'CRX FROM ADOBE'.

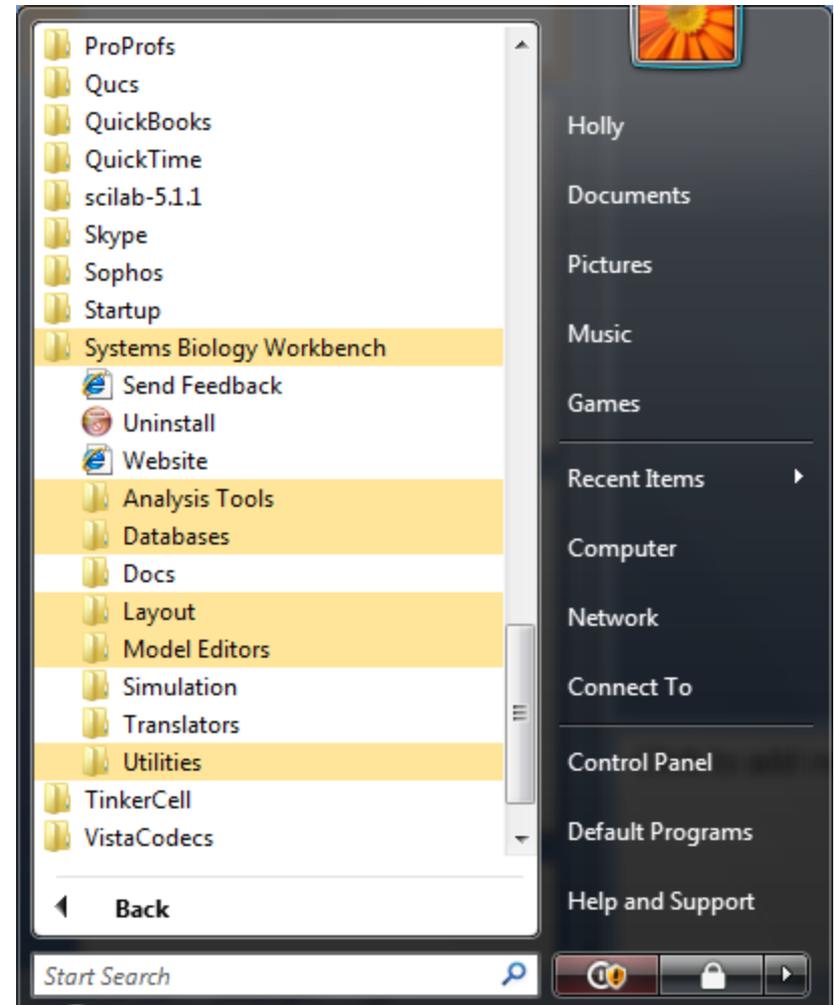
INSTALLATION FOR LINUX/OSX

From jdesigner.sf.net



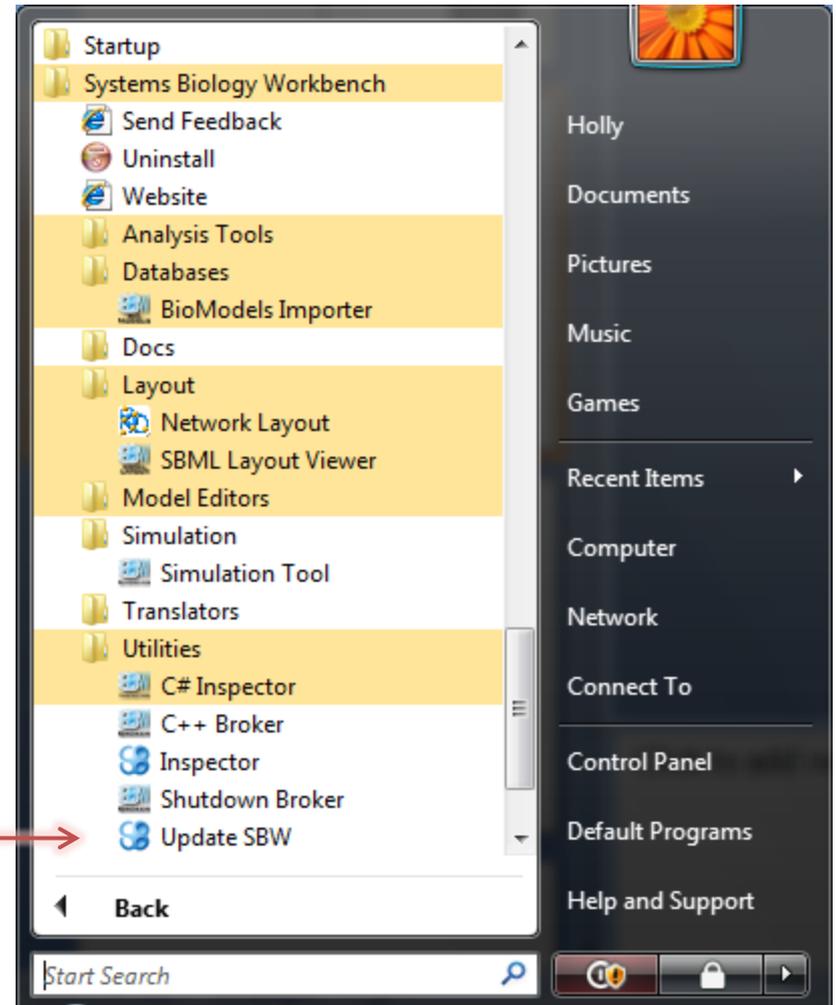
Linux/OSX is not the fully version due to porting difficulties. **Recommend** using the Windows version. A pure cross-platform version may be released next year.

Systems Biology Workbench



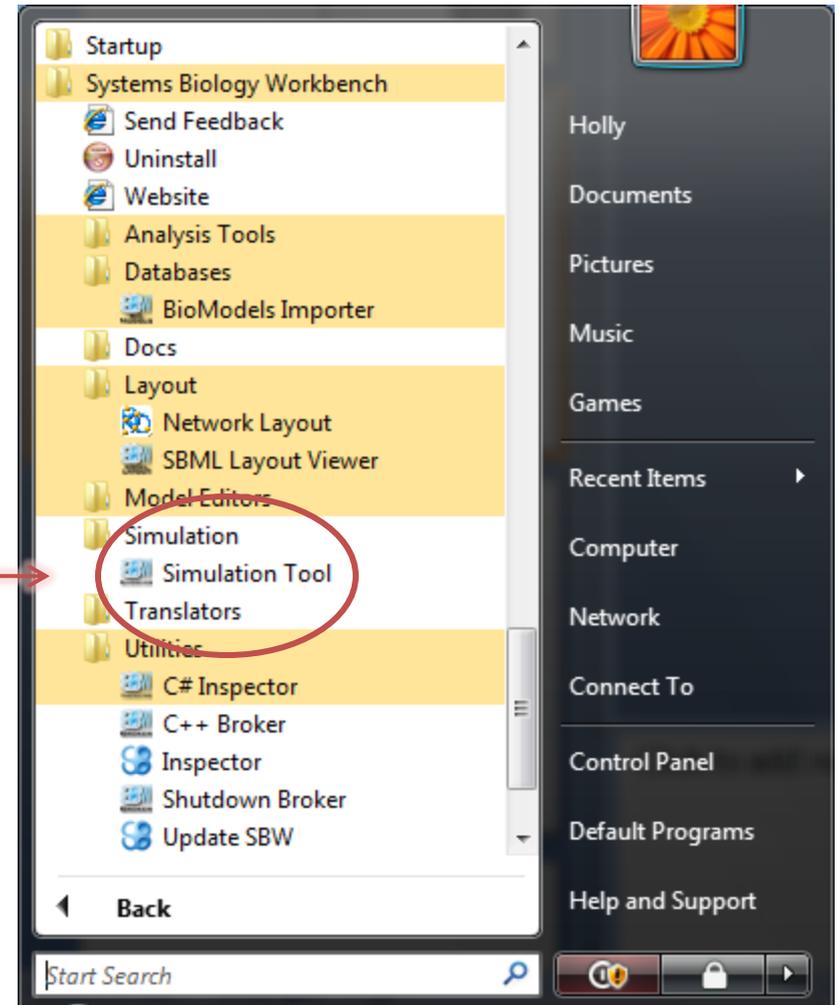
Systems Biology Workbench

Auto Update



Systems Biology Workbench

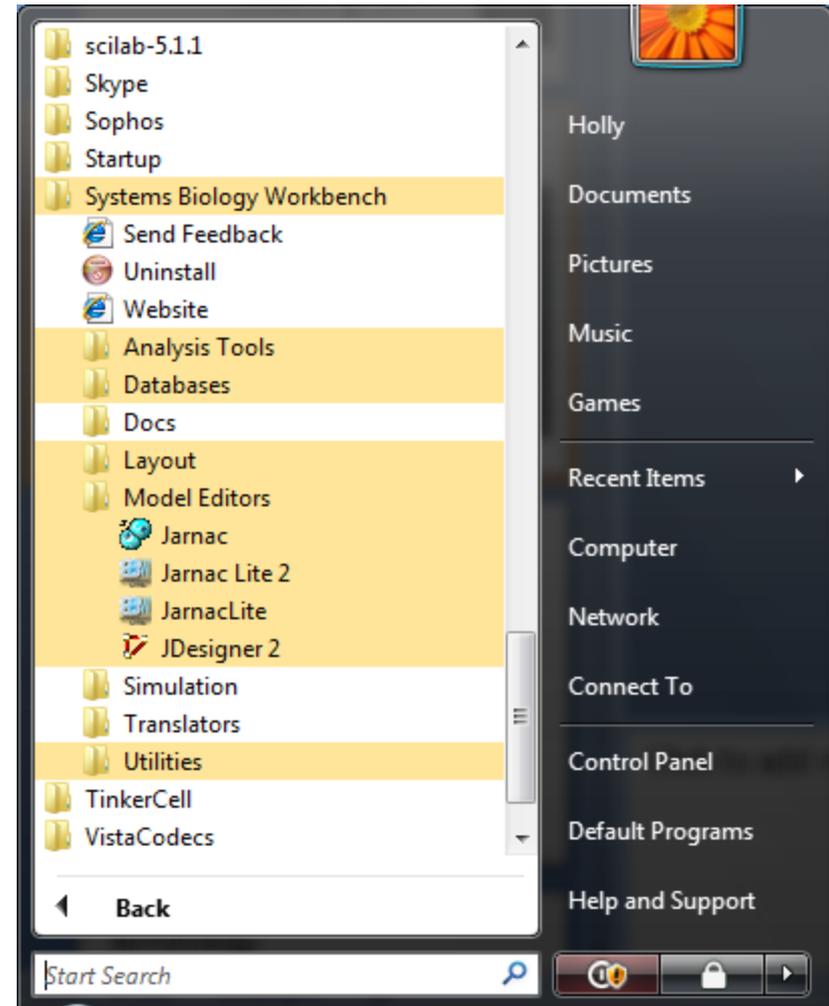
A main entry point for many users



Systems Biology Workbench

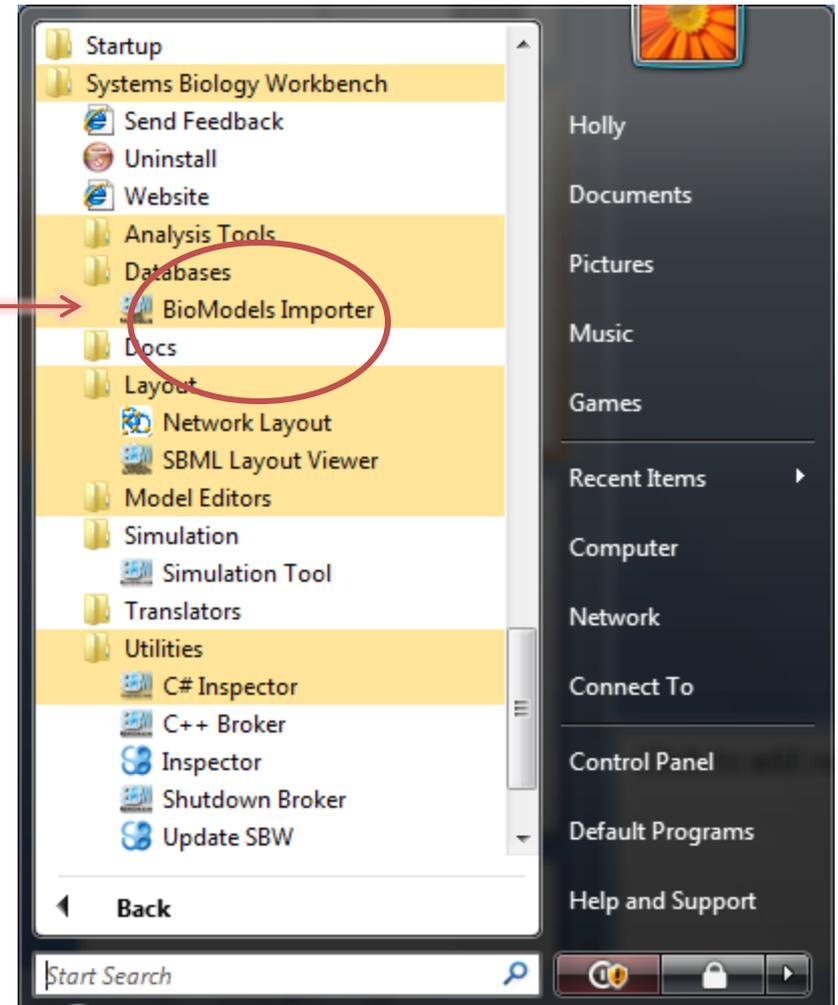
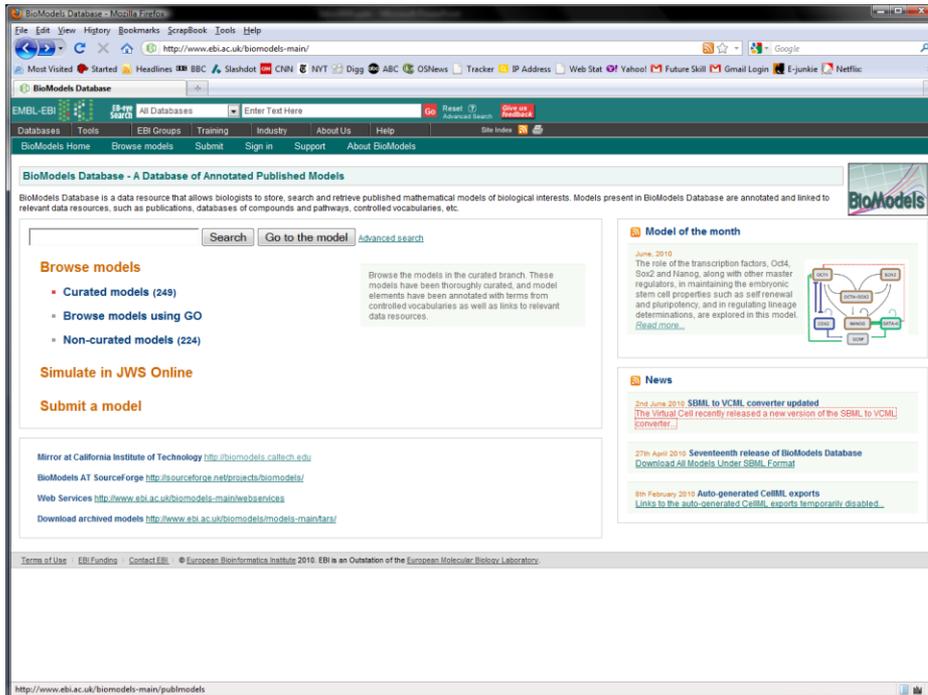
Other possible entry points

- Jarnac:** Script based modeling tool
- JarnacLite:** Small version of above
- JDesigner:** Visual design tool



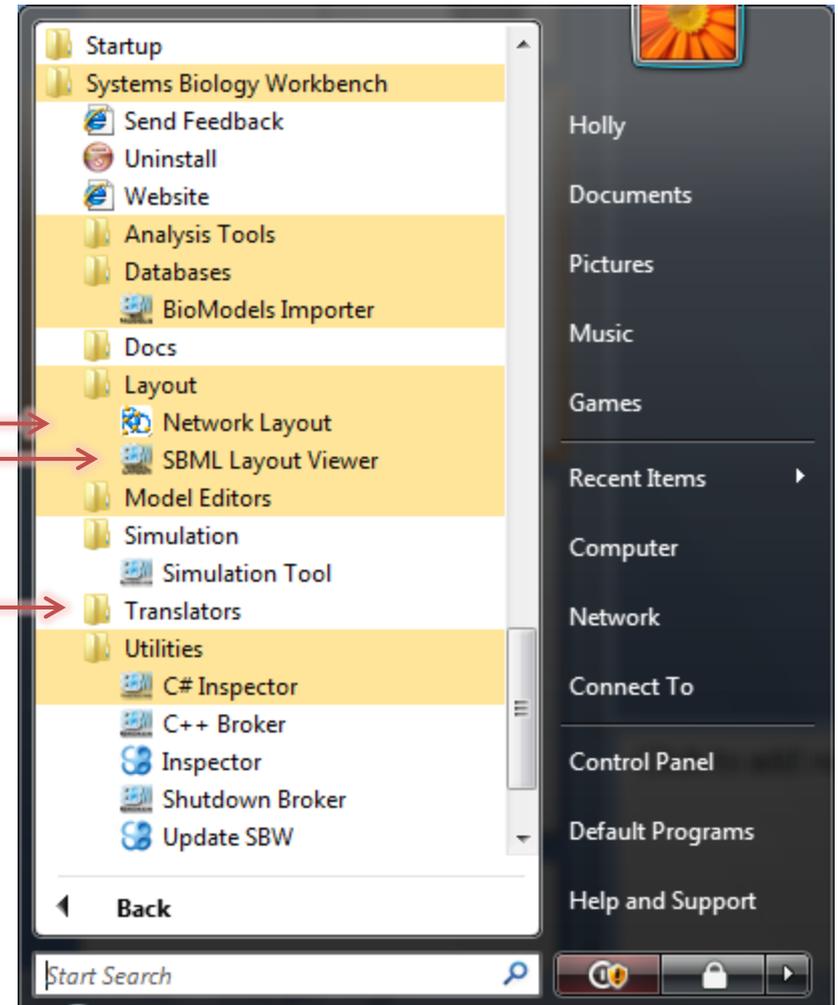
Systems Biology Workbench

Access to biomodels



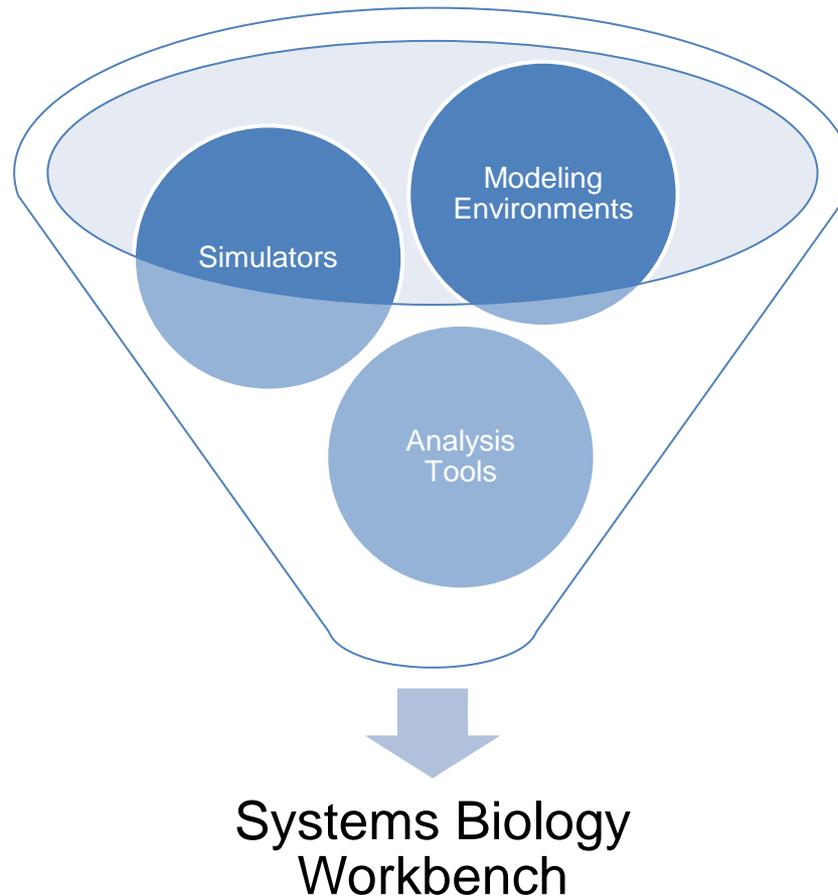
Systems Biology Workbench

Layout networks
General Network Viewer
Models Translators to:
Matlab, C, Java, C#, Jarnac,
etc

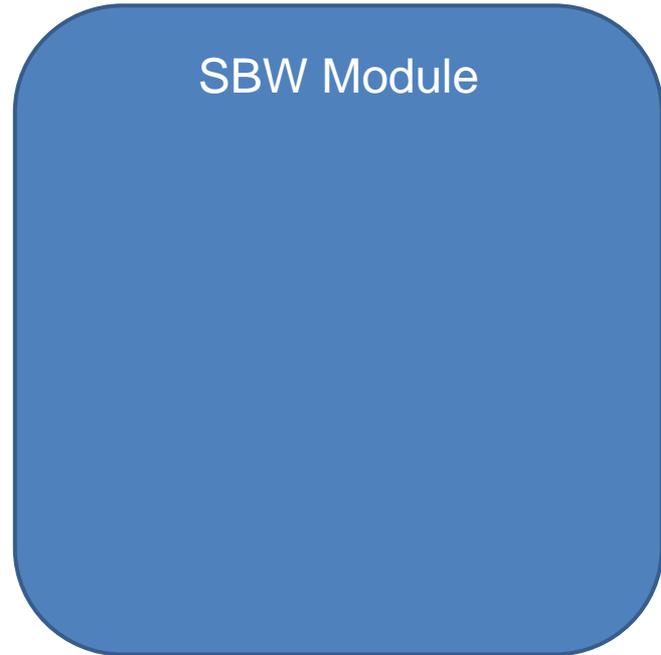
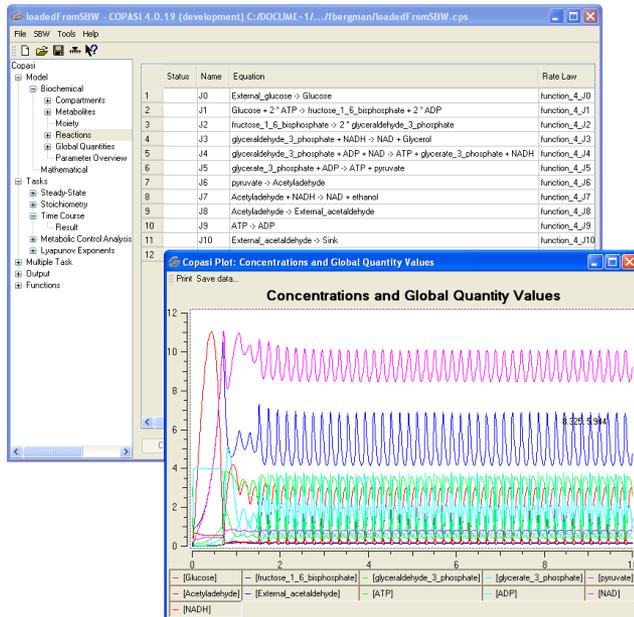


Systems Biology Workbench

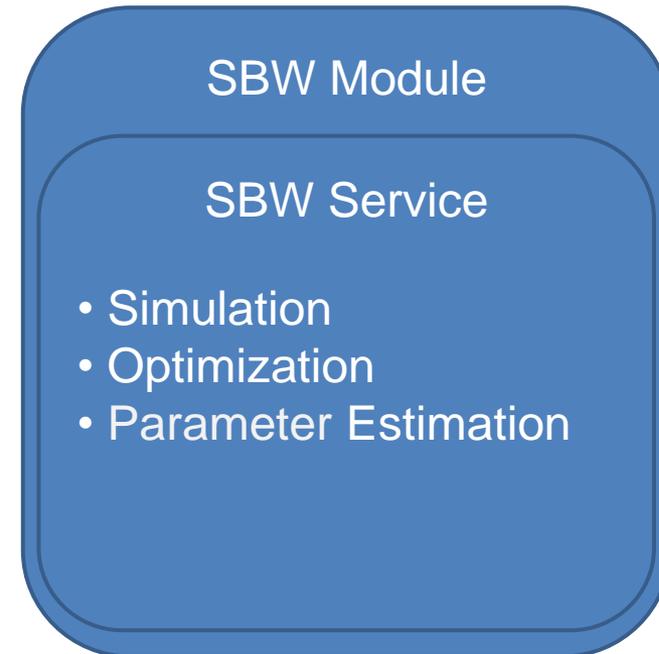
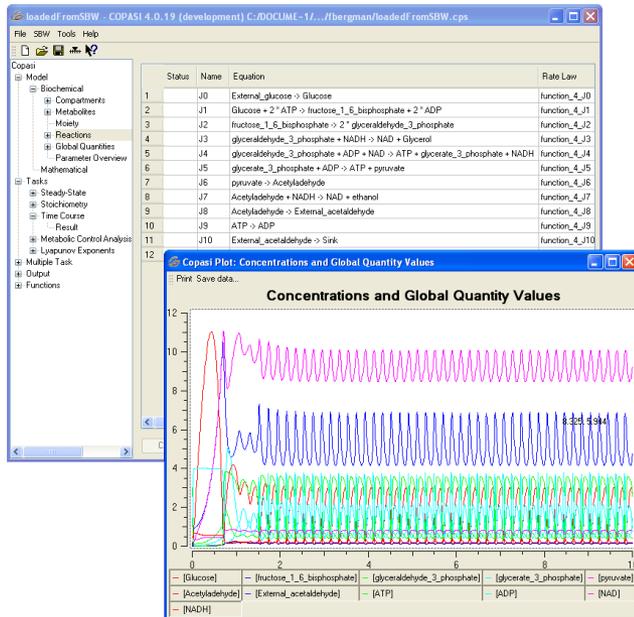
Collection of integrated tools.



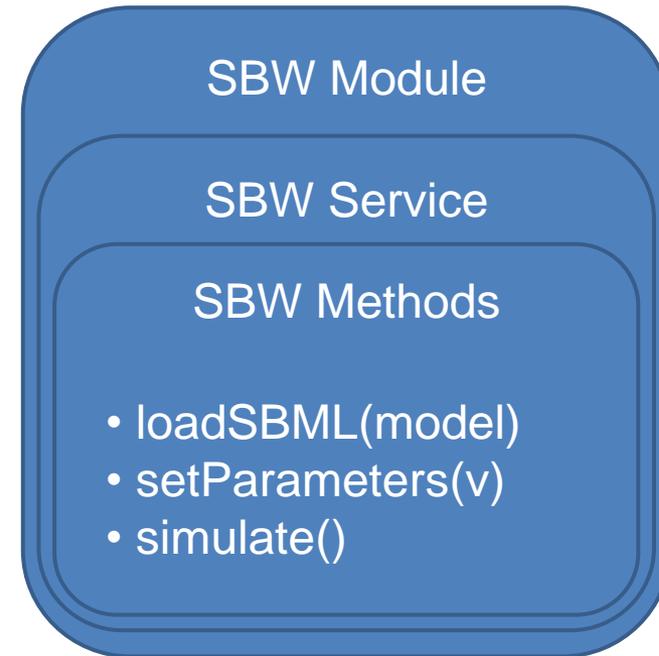
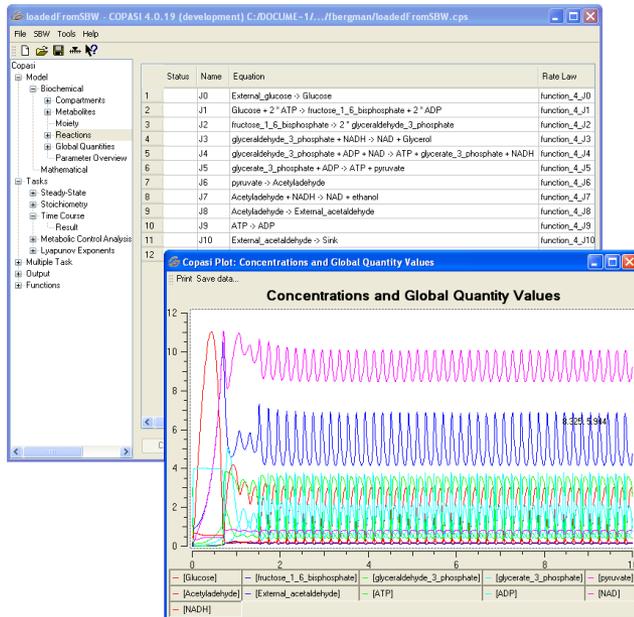
Terminology



Terminology



Terminology

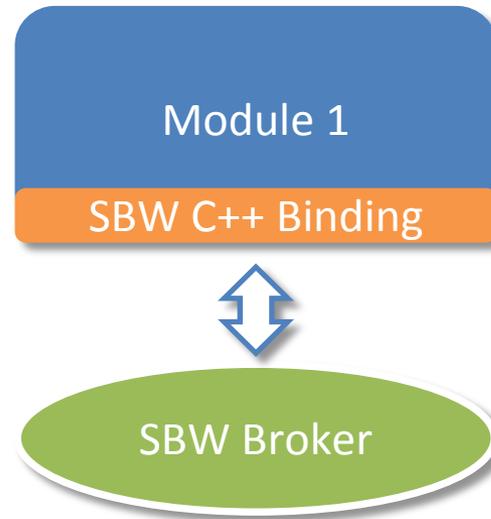


Behind the Scenes

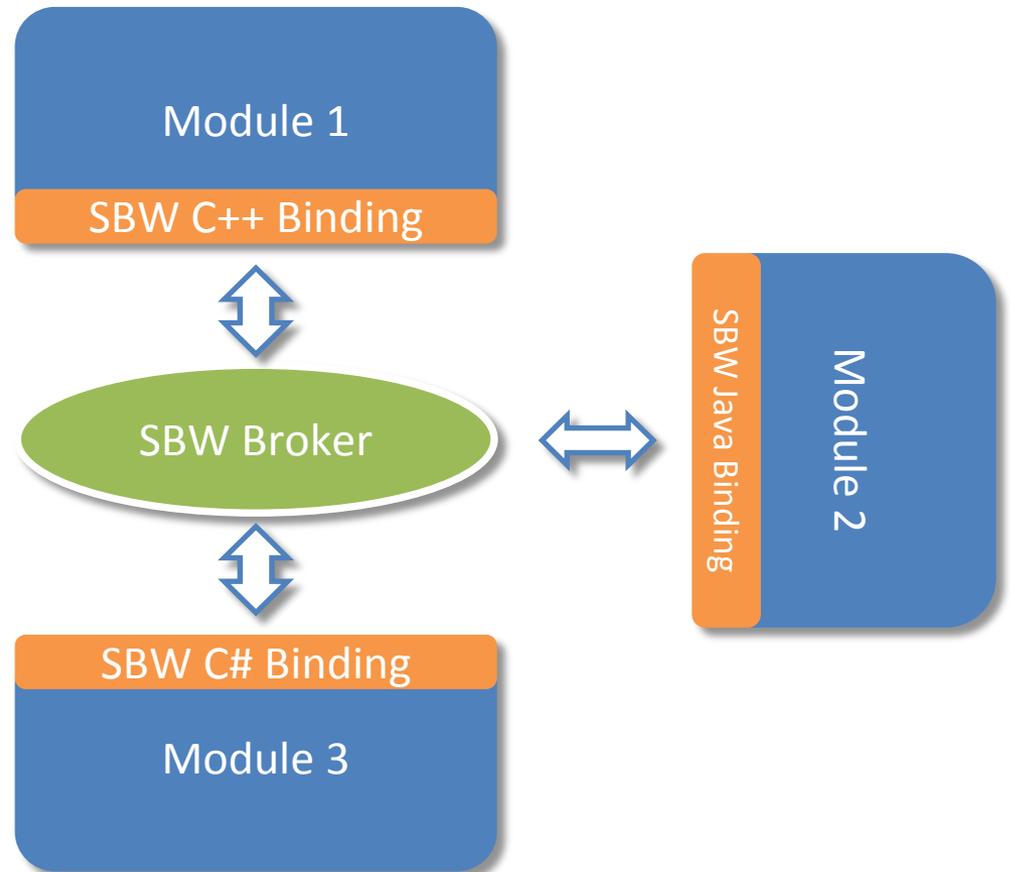
Module 1

SBW C++ Binding

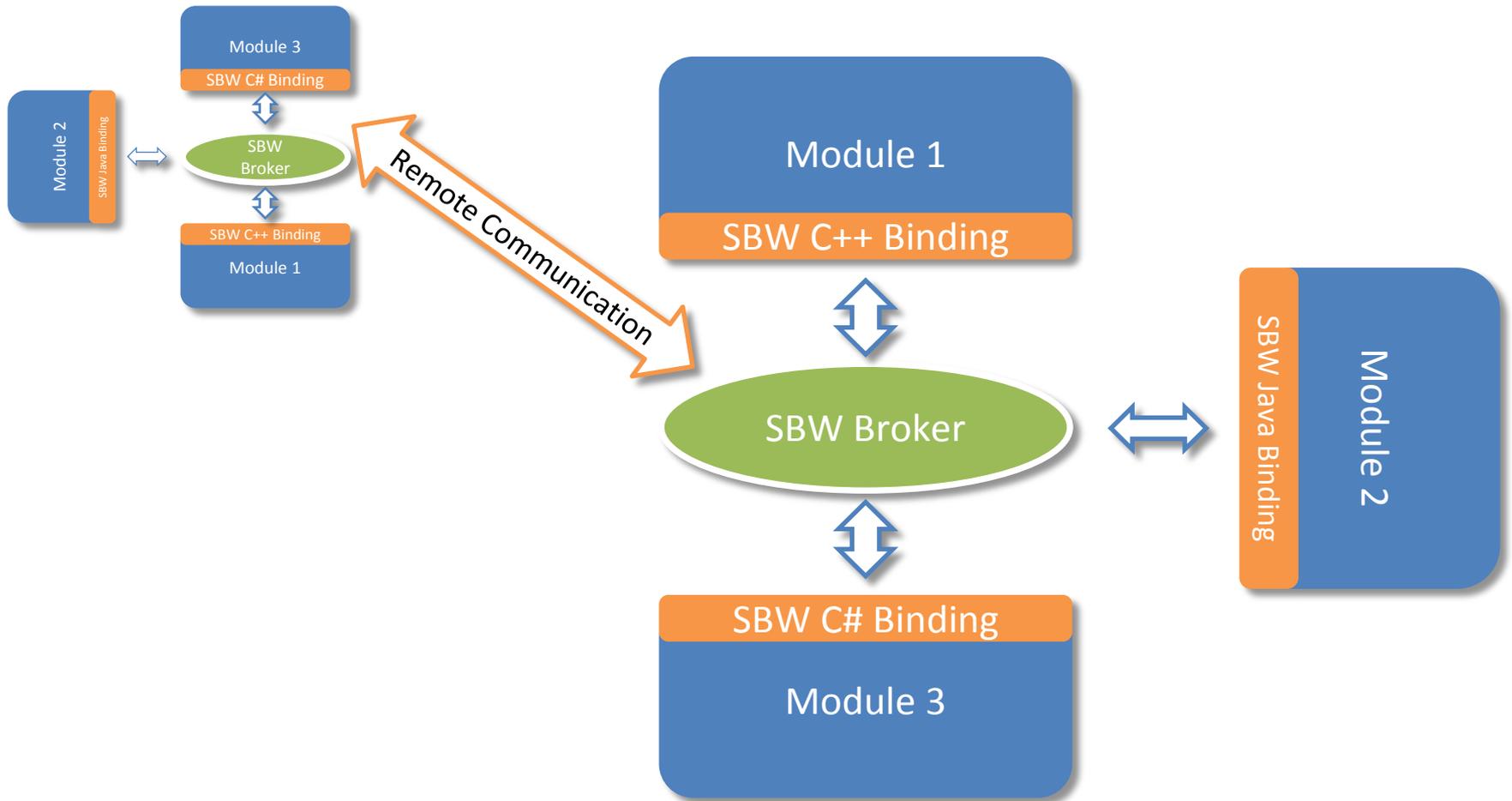
Behind the Scenes



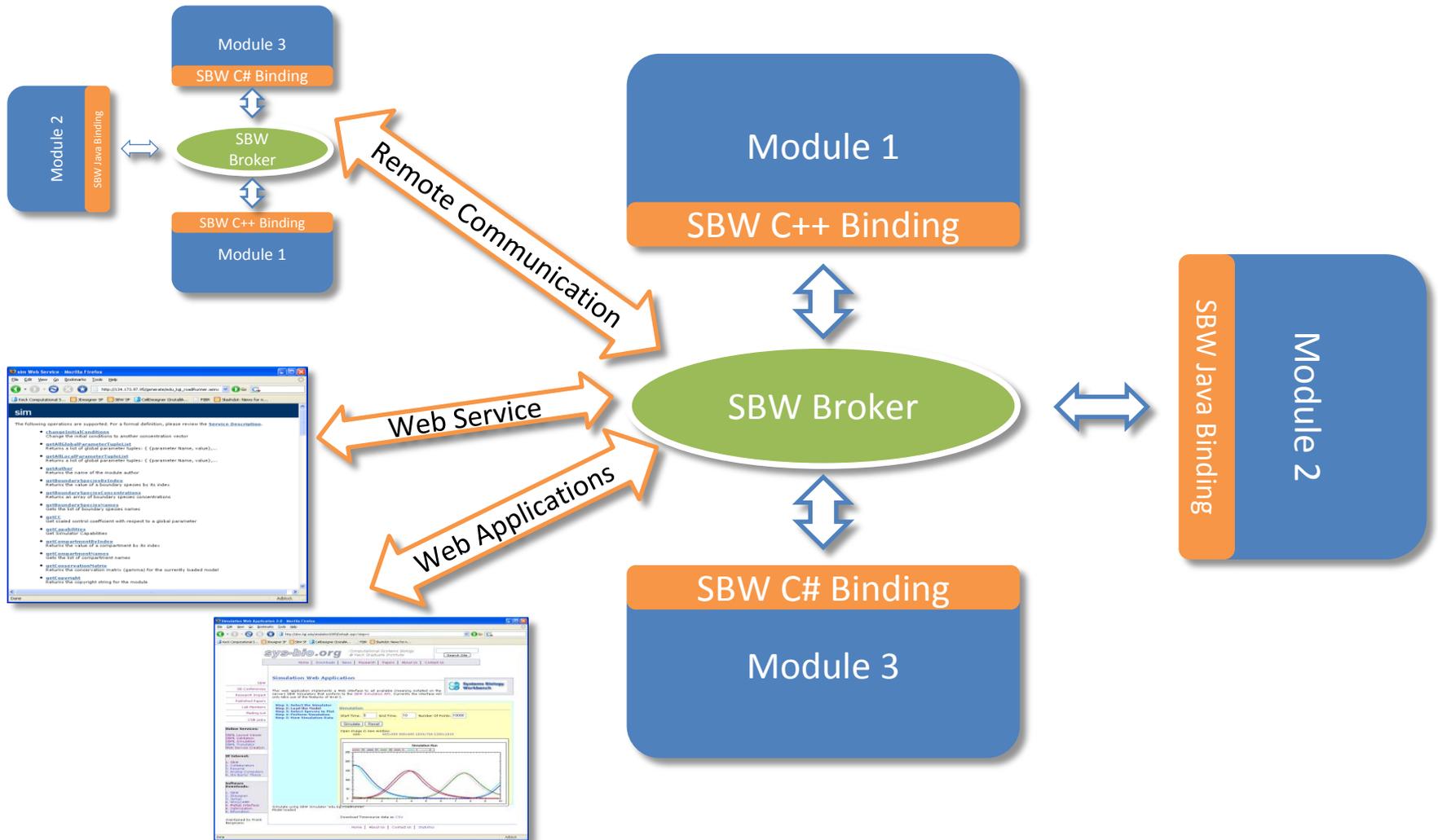
Behind the Scenes



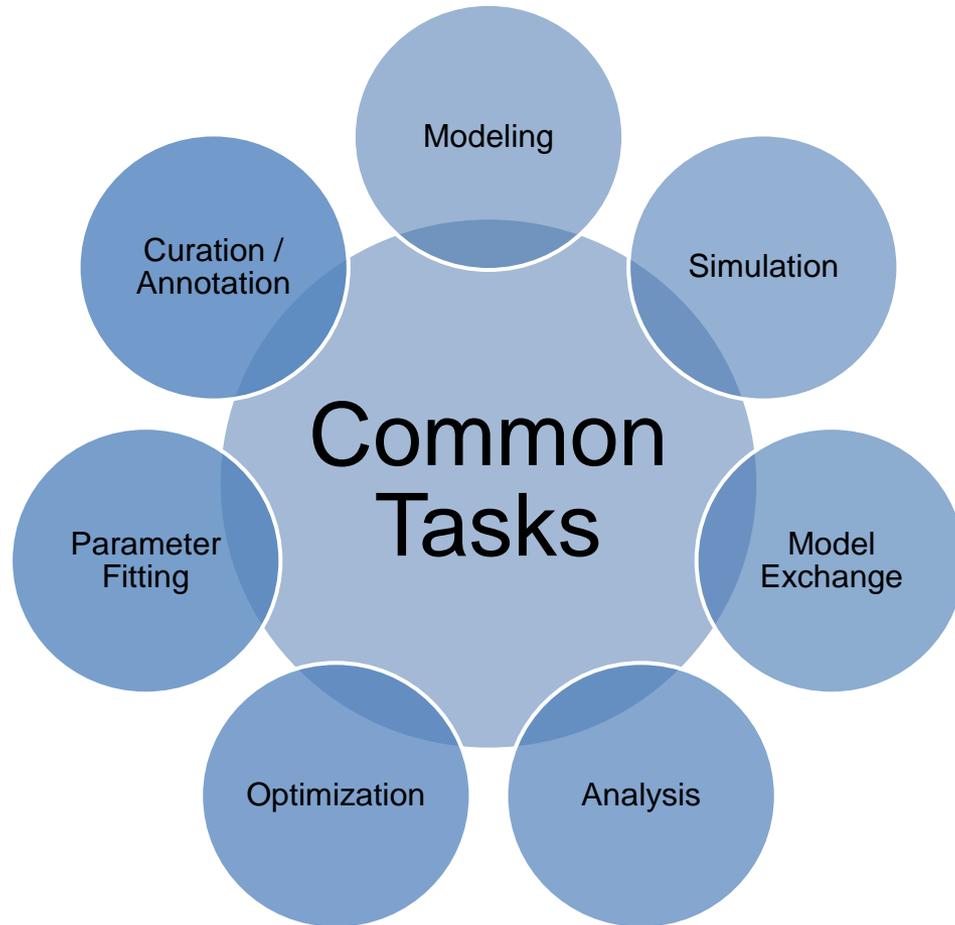
Behind the Scenes



Behind the Scenes



Motivation



Modular Approach

SBML Support

Modular Approach

SBML
Support

LAPACK
Module

Modular Approach

Structural Analysis

SBML
Support

LAPACK
Module

Modular Approach

Simulator

Structural
Analysis

LAPACK
Module

SBML
Support

Modular Approach

Modeling Environment

Simulator

Layout
Module

Further
Analysis
Modules

SBML
Support

LAPACK
Module

Structural
Analysis

SBML
Layout
Support

How is interchange accomplished?

By Community Agreed Standards

SBML (Systems Biology Markup Language): de facto standard for representing cellular networks. A large number (>200) of tools support SBML.

CellML: Stores models in mathematical form, therefore is quite general, but biological information is lost. Not possible to reconstruct network. Less than a hand-full of tools support CellML

SBGN: A proposed standard for visually representing cellular networks. No persistent format has yet been devised which limits its use in software.

Open but 'non-standard' Representations

Jarnac and JarnacLite: Script based format for describing networks, can be easily translated to and from SBML.

Antimony: Script based modular format (extension of Jarnac) for describing networks, can be easily translated to and from SBML and Jarnac. (and soon CellML)

BioNetGen: Rule based scripting language for describing networks

SBML

The screenshot shows the SBML.org website in a Mozilla Firefox browser window. The browser's address bar displays the URL http://sbml.org/Main_Page. The website header features the SBML.org logo and the title "The Systems Biology Markup Language". A navigation menu includes links for News, Documents, Downloads, Forums, Facilities, Community, Events, and About, along with a search bar. The main content area is divided into several sections:

- Welcome:** A paragraph introducing SBML as a computer-readable format for biological processes, suitable for metabolism, cell signaling, and other processes, evolving since 2000.
- For the curious:** A section with a question mark icon, advising users to read the [introduction](#) and browse [mailing lists](#) to understand SBML.
- For modelers:** A section with a bar chart icon, pointing to a [software guide](#) listing over 180 systems and the [BioModels Database](#).
- For software developers:** A section with a laptop icon, directing users to the [basic introduction](#) and [SBML specifications](#), and mentioning [libSBML](#).

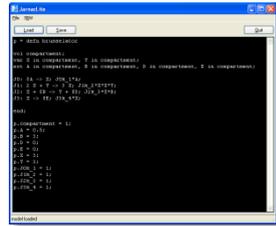
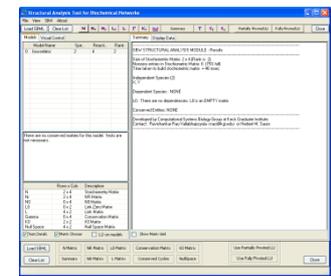
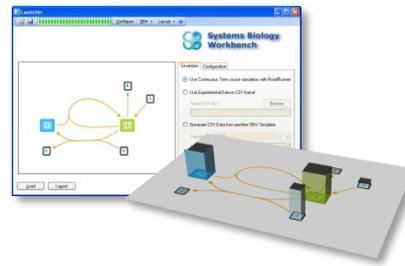
Below these sections, a paragraph invites users to sign up for news updates via [RSS feed](#), [Twitter feed](#), or [mailing lists](#), and to contribute to [community efforts](#) and display the [SBML logo](#). A final paragraph acknowledges support from [multiple agencies and organizations](#) and [major contributors](#).

The right sidebar contains news updates:

- SBML News:**
 - SBMLToolbox 3.1.2!** (27 Apr.'10): A minor bug-fix release of the free MATLAB toolbox for SBML.
 - SBMLToolbox 3.1.1!** (12 Apr.'10): A minor bug-fix release of the free MATLAB toolbox for SBML.
 - Older news ...**
- Community News:**
 - COPASI 4.6 Released** (22 Jul.'10): The new stable release of COPASI adds support for events, new stochastic algorithms, and SBML L2v4.
 - CellDesigner 4.1!** (30 Jun.'10): CellDesigner is a full-featured modeling environment with a GUI. This release adds SBML L2v4, SABIO-RK, MIRIAM, PANTHER, SBGN and other support.
 - Cain 1.4 released!** (31 May.'10): Cain is a stochastic simulator with highly efficient implementations of many methods.
 - Older news ...**

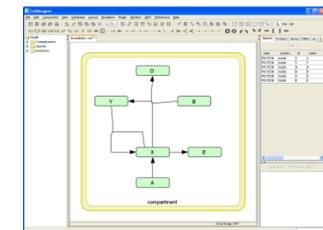
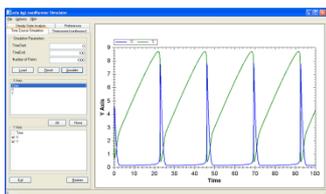
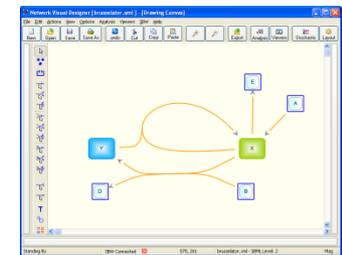
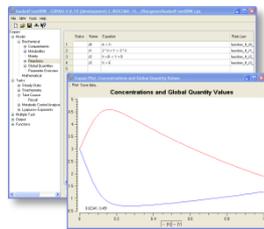
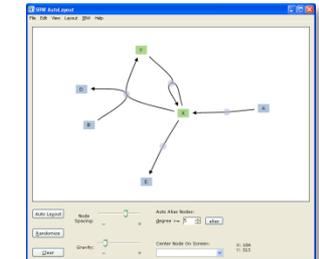
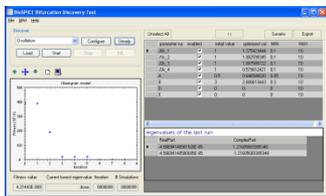
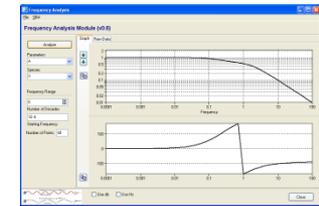
At the bottom of the page, there are social media sharing options (SHARE, Facebook, Twitter, Email) and a SourceForge logo.

SBW Menu

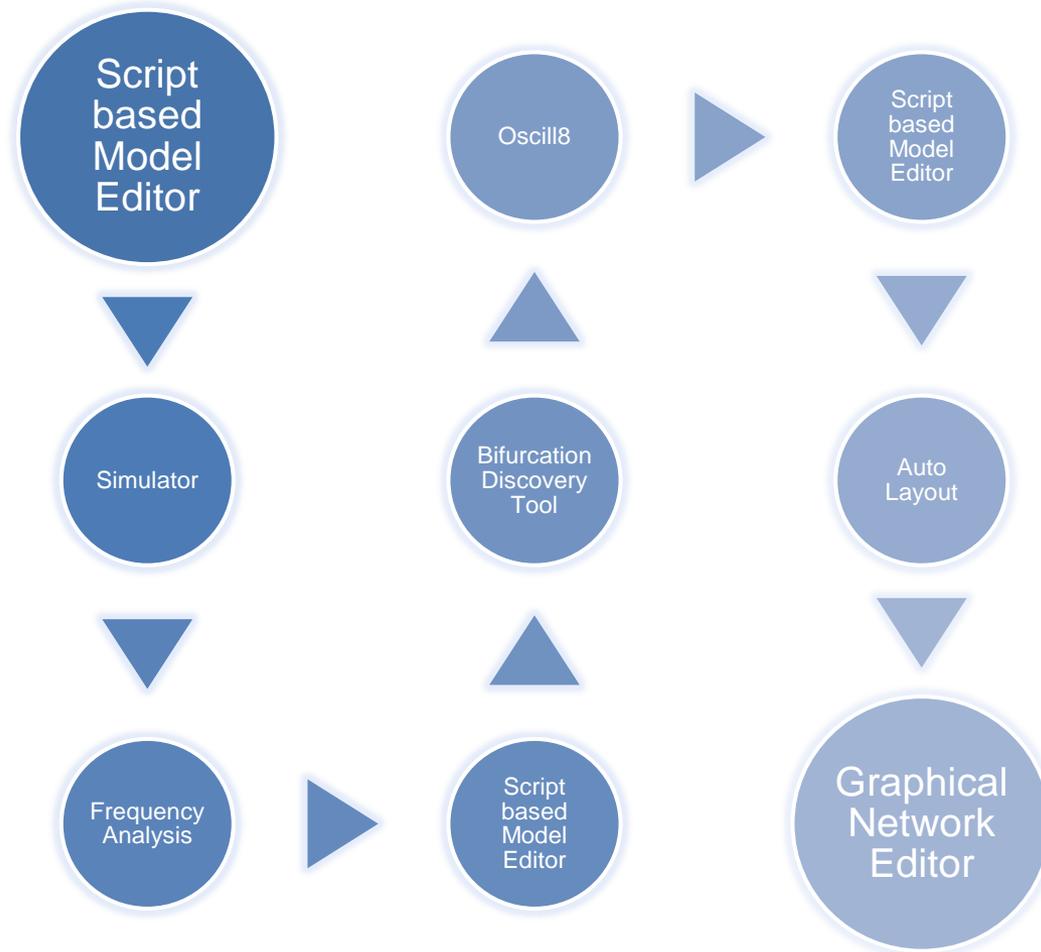


SBW

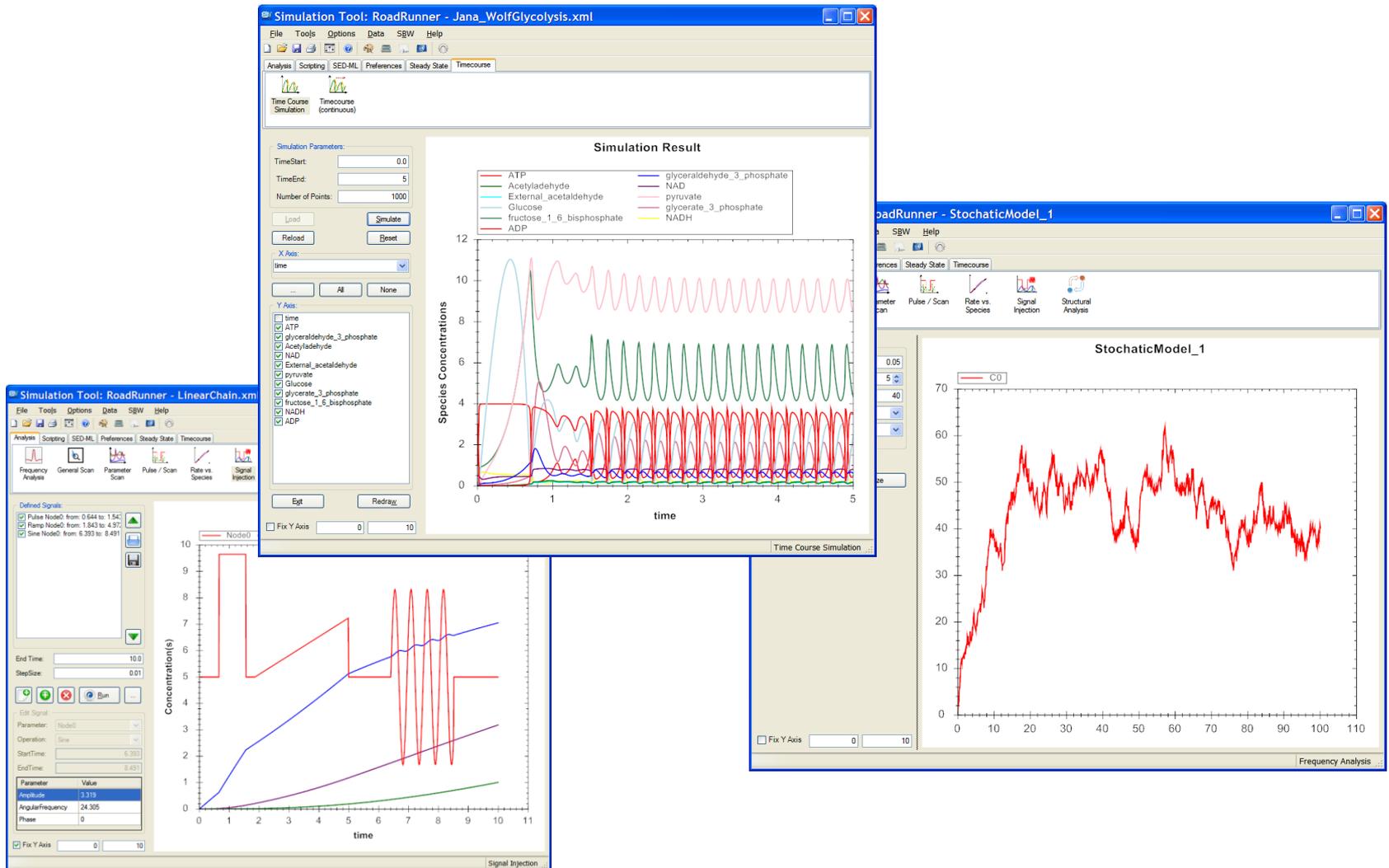
- Bifurcation Discovery Tool
- Chemical_Langevin_Equation Simulation Service
- COPASI (SBW Dev. Version)
- CVODE Simulation Service
- Dizzy Simulation Service
- edu.kgi.roadRunner Simulation Service
- Frequency Analysis Module
- Gibson_NRM Simulation Service
- Gillespie_DM Simulation Service
- Gillespie_FRM Simulation Service
- GillespieGUI
- JacobianViewer
- Jarnac Simulation Service
- JDesigner
- Layout Network
- LSODA Simulation Service
- Oscill8 GUI
- Save Model as Matlab ODE Function File
- Save Model as Matlab SimuLink Function File
- SBML layout reader (GUI)
- Simulate 3D (OpenGL)
- Structural Analysis Tool



Example Workflow



General Simulation Tool



General Simulation Tool

Gillespie Library

Structure Analysis

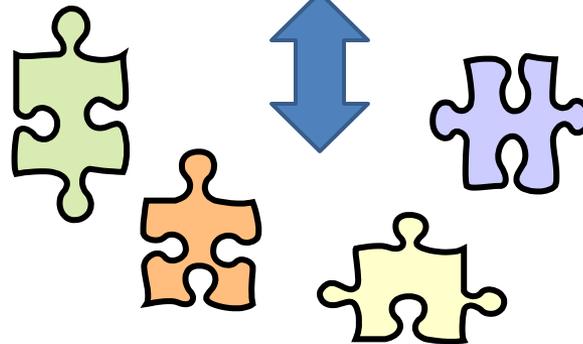
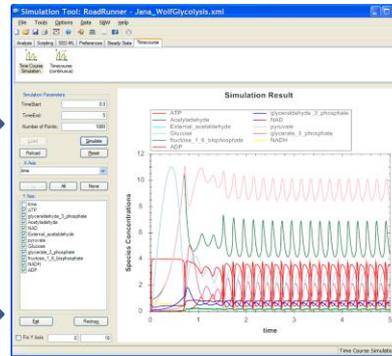
Biomodels DB

Simulator RoadRunner

SBML Support

Python Plugin

To SBW



Other Types of Plugins, eg GUI (See next slide)

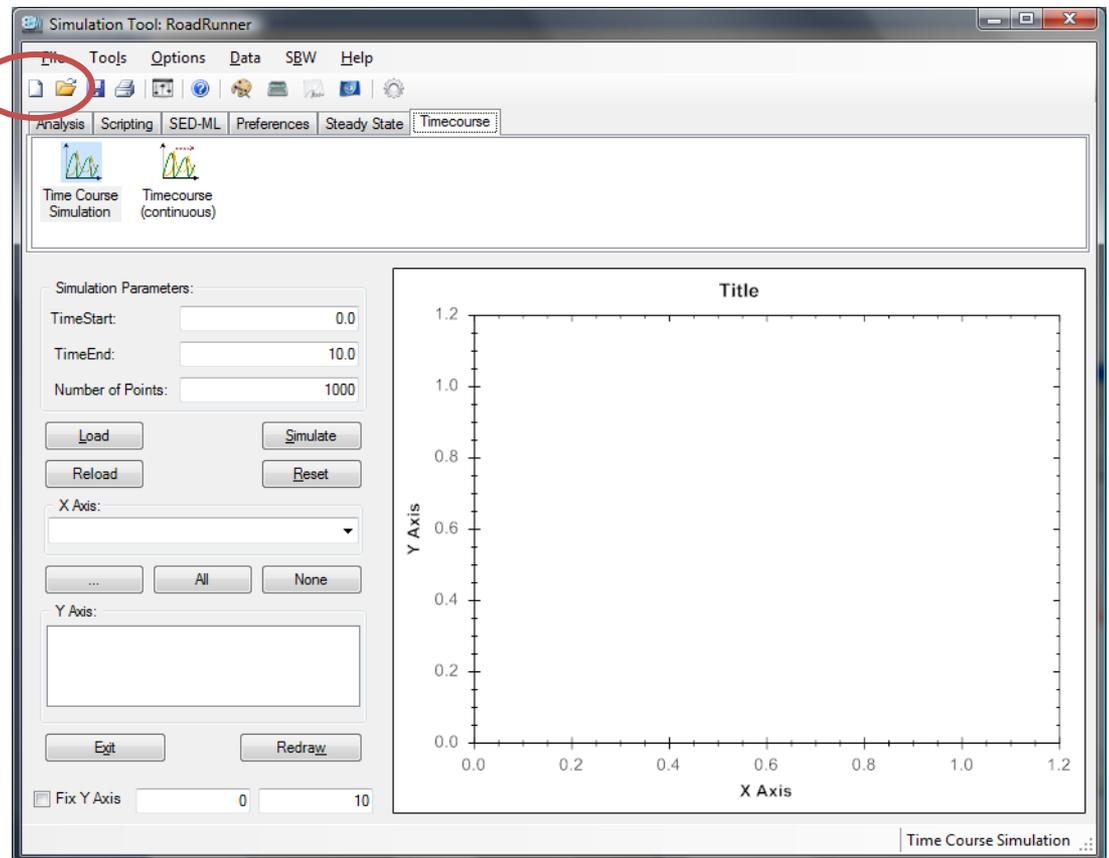
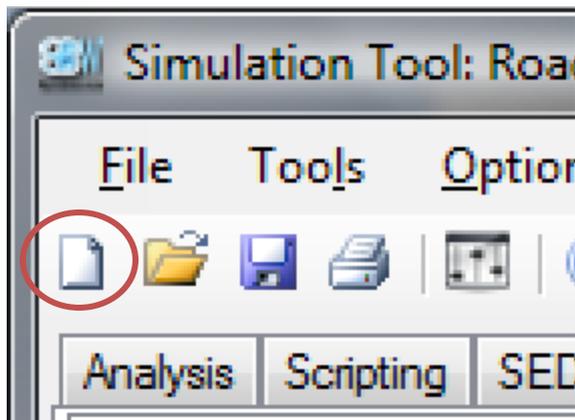
General Simulation Tool

Current Set of Plugins:

1. Time Course Simulation
2. Steady State including MCA
3. Parameter Scans
4. Signal Injection
5. Frequency Analysis
6. Analysis of Stoichiometry Matrix
7. SED-ML (describing simulation experiments (experimental!))
8. Species versus rate tool
9. Python Scripting with access to the internal object model

Try a Simple Simulation

1. Start the Simulation Tool
2. Click on the new button (top left)



Try a Simple Simulation

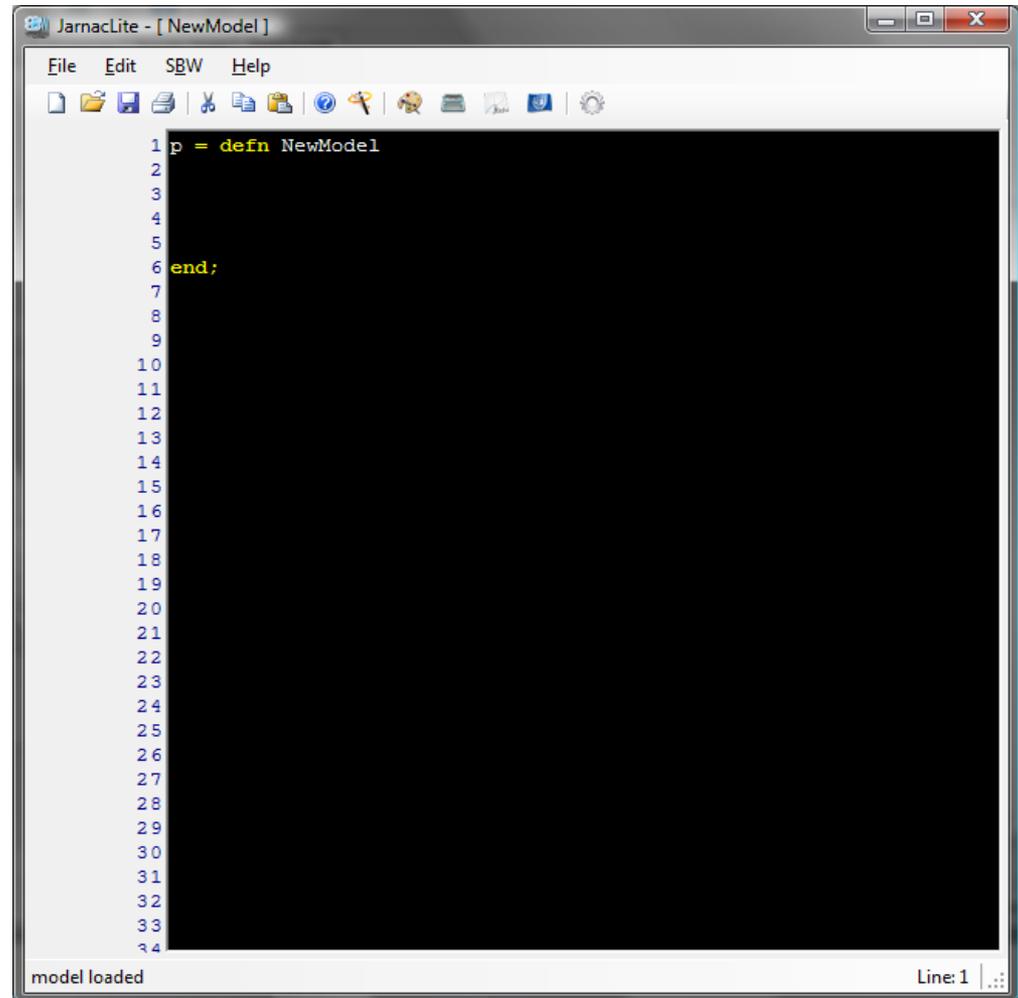
The model editing window should appear,
type the following in the window:

```
p = defn cell
    S1 -> S2; k1*S1;
    S2 -> S3; k2*S2;
end;
```

```
p.S1 = 10;
p.S2 = 0;
p.S3 = 0;
```

```
p.k1 = 0.34;
p.k2 = 1.3;
```

Make sure you hit return after
the last line!

The image shows a screenshot of a software window titled "JarnacLite - [NewModel]". The window has a menu bar with "File", "Edit", "SBW", and "Help". Below the menu bar is a toolbar with various icons. The main area is a text editor with a black background and white text. The text in the editor is:

```
1 p = defn NewModel
2
3
4
5
6 end;
7
8
9
10
11
12
13
14
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20
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```

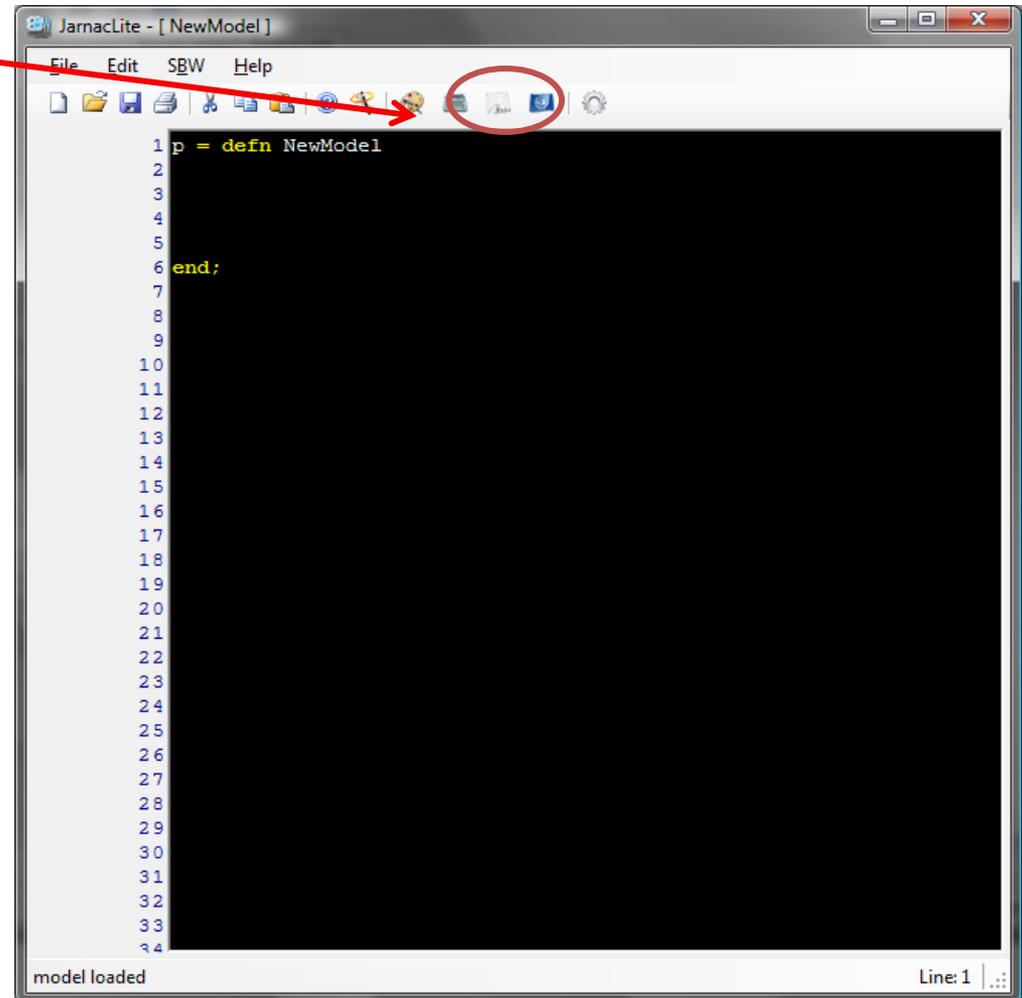
The status bar at the bottom of the window shows "model loaded" on the left and "Line: 1" on the right.

Try a Simple Simulation

Move the mode to the simulation
Tool by clicking on:

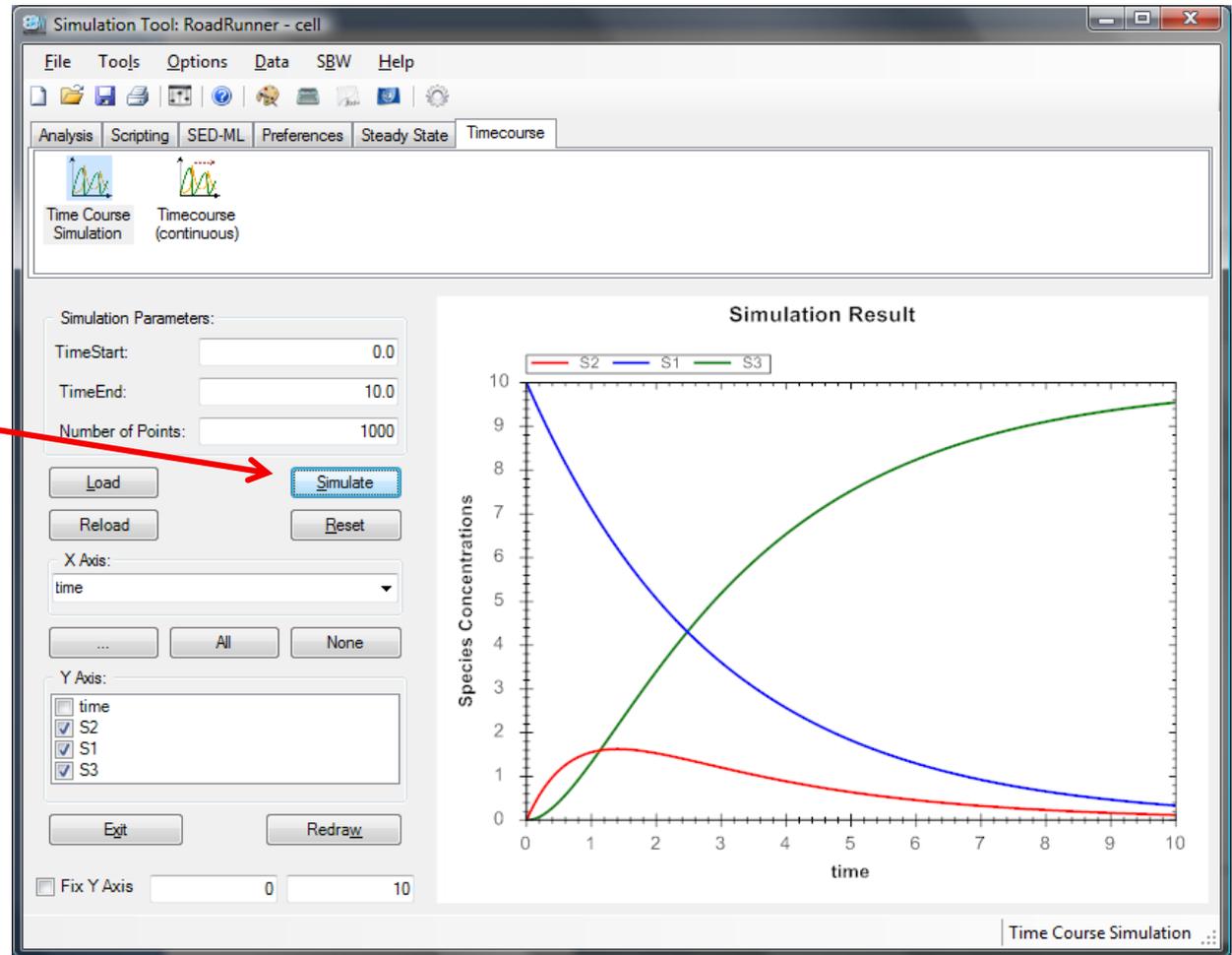


Third button from the right.



Try a Simple Simulation

Click to run simulation



Access Data

Copy simulation data to
the clipboard or load into Excel

