

Updates about SBML

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COMBINE 2012, Toronto, Canada, August 2012

outline

Brief summary of SBML for the unfamiliar

Recent development in Level 3 packages

Recent developments in the SBML Test Suite

Closing

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What are the outcomes of modeling and simulation?

Usually, there are at least two scientific outcomes:

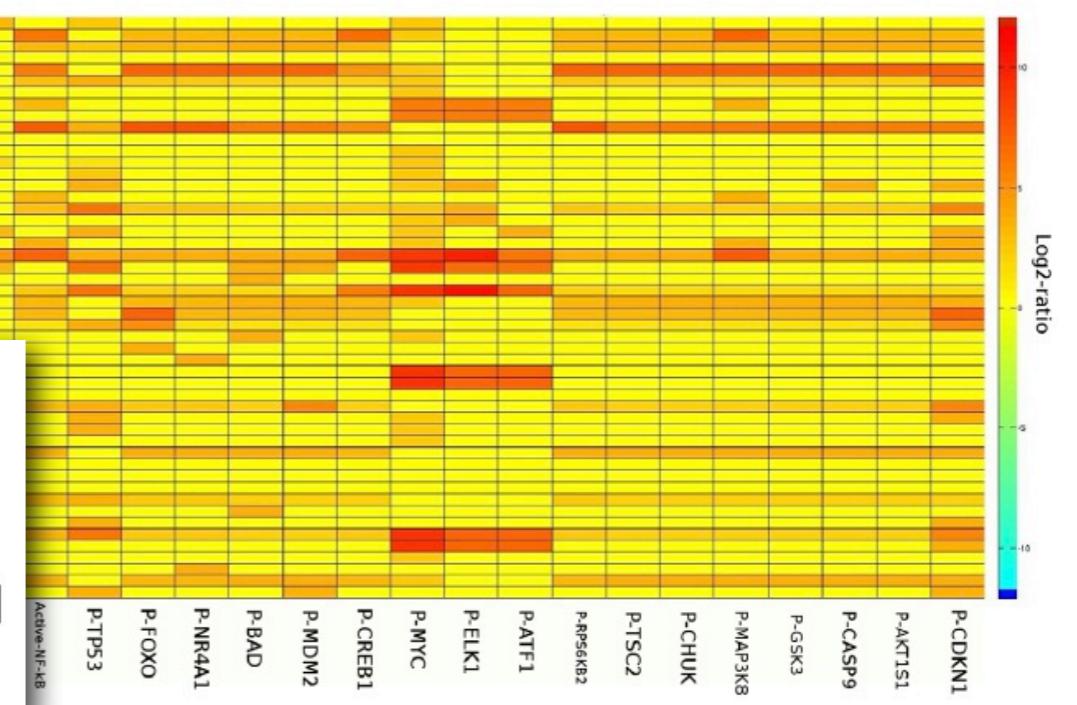
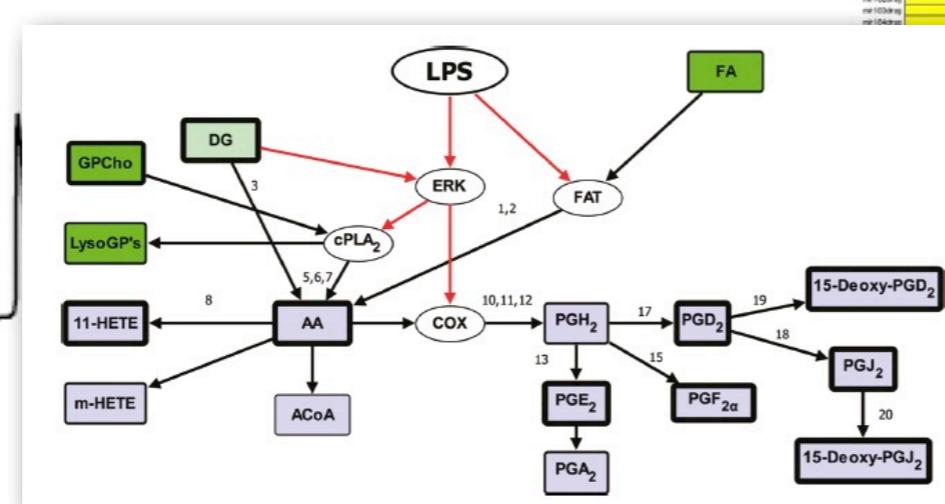
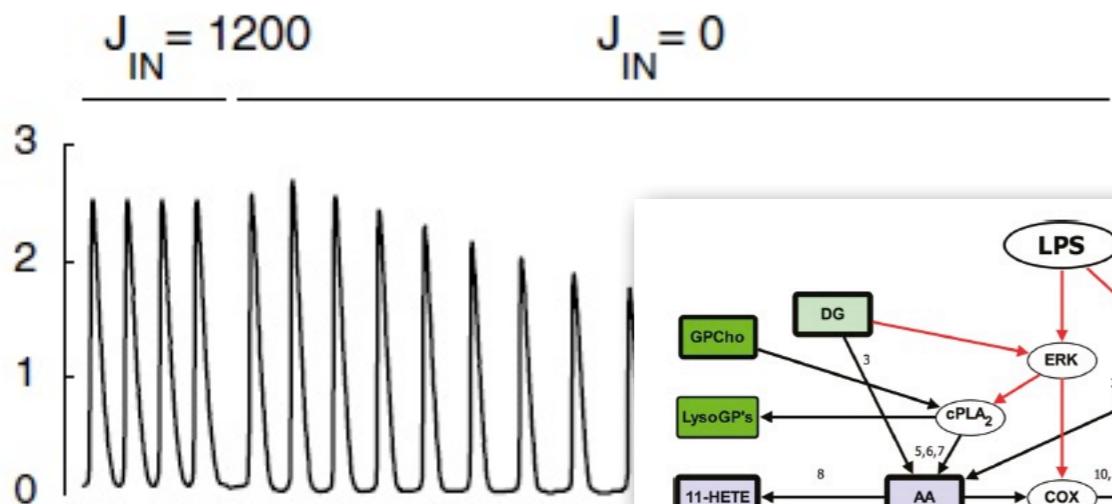
- One or more models (+ associated claims about their behaviors)
- Publication of the results (in some form)

$$dx_1/dt = -k_{12}[G]_{\text{out}}x_1 + k_{21}x_2 + k_{41}x_4 - k_{14}x_1,$$

$$dx_2/dt = k_{12}[G]_{\text{out}}x_1 - k_{21}x_2 - k_{23}x_2 + k_{32}x_3,$$

$$dx_3/dt = k_{23}x_2 - k_{32}x_3 - k_{34}x_3 + k_{43}[G]_{\text{in}}x_4,$$

$$dx_4/dt = k_{34}x_3 - k_{43}[G]_{\text{in}}x_4 - k_{41}x_4 + k_{14}x_1.$$



Models come
in many forms

Models a fundamentally important scientific work product

Models serve as **statements of our current understanding** of the phenomena being studied*

- A computational model documents your theory in a concrete form

Model can—

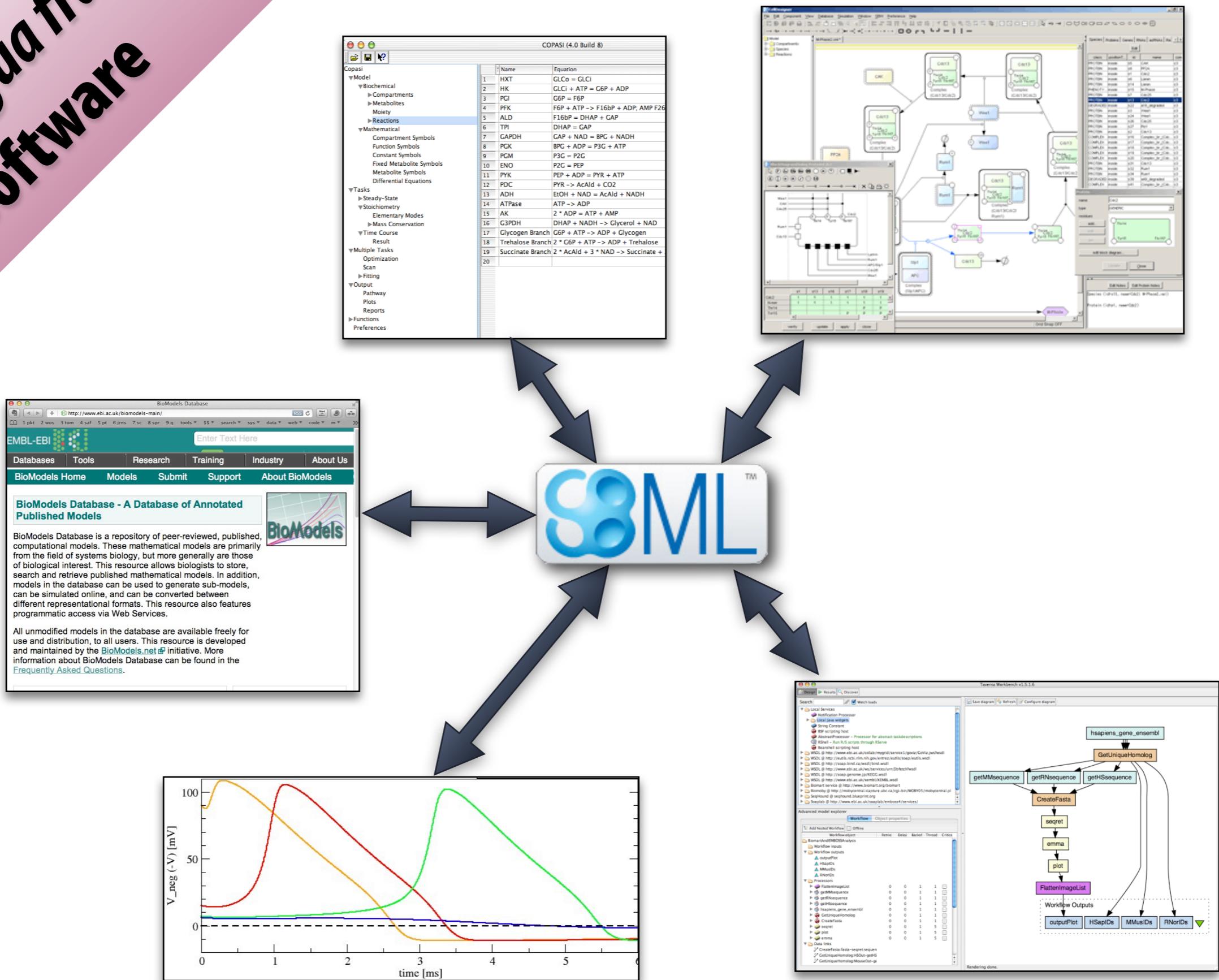
- **Reduce ambiguity** in communication
- Offer a **concrete framework** for adding new data and theories
- **Support direct evaluation** of relationships between theories



Different tools ⇒ different representation languages

Communication is better with interoperable data formats

SBML: a lingua franca for software



SBML = Systems Biology Markup Language

Format for representing computational models of biological processes

- Data structures + usage principles + serialization to XML

Neutral with respect to modeling framework

- E.g., ODE, stochastic systems, etc.

Development started in 2000, with first specification distributed in 2001

The **process** is central

- Called a “reaction” in SBML
- Participants are pools of entities (**species**)

Models can further include:

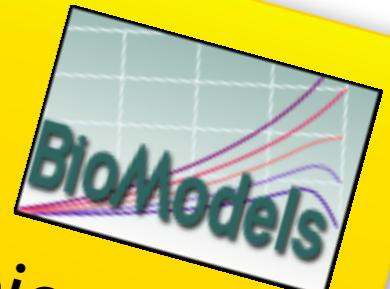
- Other constants & variables
- Compartments
- Explicit math
- Discontinuous events
- Unit definitions
- Annotations

Basic SBML concepts are fairly simple

Today: spatially homogeneous models

- Metabolic network models
- Signaling pathway models
- Conductance-based models
- Neural models
- Pharmacokinetic/dynamics models
- Infectious diseases

Find examples in
BioModels Database
<http://biomodels.net/biomodels>



Coming: SBML Level 3 packages to support other types

- E.g.: Spatially inhomogeneous models, also qualitative/logical

Scope of SBML encompasses many types of models

Find software in the SBML Software Guide

Main Page – SBML.org

http://sbml.org/Main_Page Reader Google

 The Systems Biology Markup Language

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Welcome to the portal for the **Systems Biology Markup Language (SBML)**, a free and open interchange format for computer models of biological processes. SBML is useful for models of metabolism, cell signaling, and more. It has been in development by an international community since the year 2000.

For the curious
 What is SBML? Read our [introduction](#), then perhaps browse the [mailing lists](#) to glimpse what's happening with SBML today.

For modelers
 Looking for software that supports SBML? Our [software guide](#) lists over **220** systems. Are you instead looking for models? Visit [BioModels Database](#), where you can find hundreds!

For software developers
 Interested in supporting SBML in your software? Read our [basic introduction](#) and then the [SBML specifications](#) to understand how to use SBML. After that, you may want to look at [libSBML](#).

No matter how you use SBML, we invite you to sign up for news updates either through our [RSS feed](#), our [Twitter feed](#), or one of the [mailing lists](#), and get involved with [community efforts](#) to help keep improving SBML. You can also call attention to your project's support of SBML by displaying the [SBML logo](#).

SBML would not have been possible without support from [multiple agencies and organizations](#), as well as intellectual contributions from many motivated individuals, including the [major contributors](#) who are shaping SBML Level 3.

SBML News

COMBINE 2011 
(14 Jun. '11) Registration is now open for [COMBINE 2011](#), being held in Heidelberg, DE, on Sep. 3-7.

SBML Test Suite updated 
(6 Jun. '11) Changes include addition of SBML L3v1 Core test cases, SED-ML files, and updates to the online interface.

[Older news ...](#)

Community News

PRISM 4.0 released 
(3 Jul. '11) [PRISM](#) 4.0 is a probabilistic model checker that supports SBML input.

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(29 Jun. '11) [MatCont](#) is a MATLAB package for studying parameterized continuous and discrete dynamical systems.

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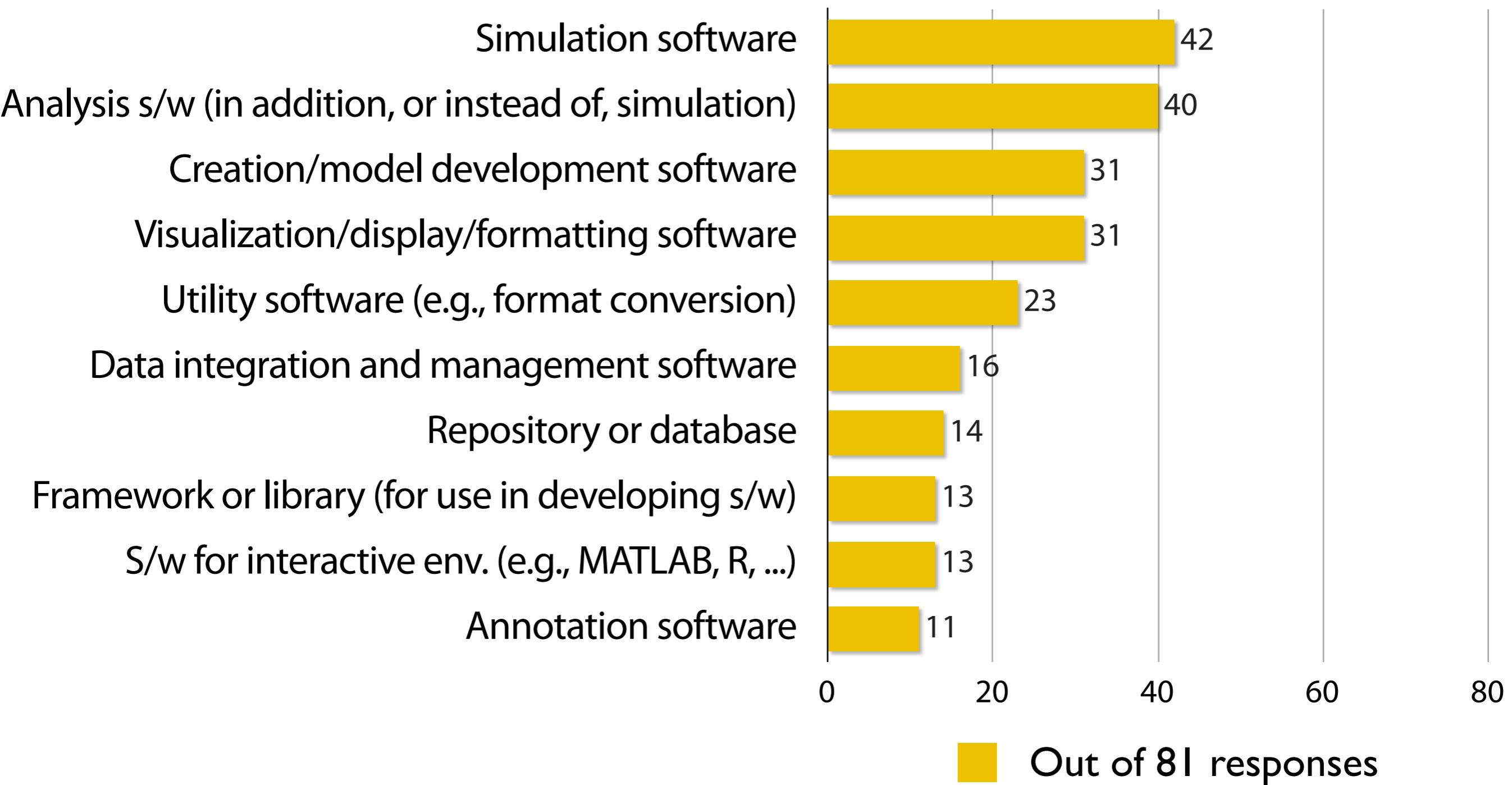
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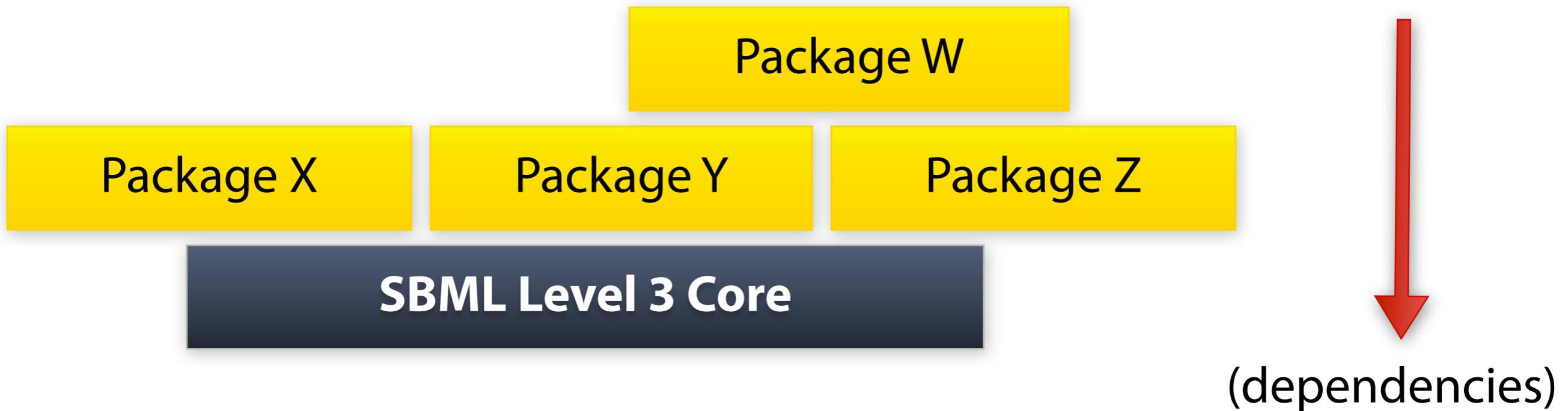
Find SBML software

Results of 2011 survey of SBML-compatible software

Question: *Which of the following categories best describe your software?
(Check all that apply.)*



SBML Level 3: Supporting more categories of models



An **SBML Level 3 package** adds constructs & capabilities

- Models declare which packages they use
- Applications tell users which packages they support

Package development can be decoupled

Development process described at <http://sbml.org/Documents>

SBML Development Process

The screenshot shows a web browser window with the following details:

- Title Bar:** Documents/SBML Development Process – SBML.org
- Address Bar:** http://sbml.org/Documents/SBML_Development_Process
- Toolbar:** Includes icons for Reader, Word, Print, Back, Forward, Stop, Refresh, and others.
- Menu Bar:** 1 pkt, 2 wos, 3 tom, 4 saf, 5 pt, 6 jrn, 7 sc, 8 spr, 9 g, tools, \$\$, search, sys, data, web, code, >>
- Header:** SBML.org The Systems Biology Markup Language
- Navigation:** News, Documents (highlighted), Downloads, Forums, Facilities, Community, Events, About, social media links (Facebook, Twitter, RSS, Google+), Google Site Search.
- Page Content:**
 - Parent pages:** SBML.org / Documents
 - ## SBML Development Process

An intrinsic aspect of SBML's development has been the adoption of a participative, community-oriented approach. In the early years of SBML, this process was highly informal. The use of SBML has grown to the point where its original, informal approach to development is no longer sufficient to meet the needs of the SBML community and the continued evolution of SBML. Beginning in 2003, the SBML Team and SBML Editors have been working to put into place a more formal organization and systematic process, one that will be less ambiguous and subjective and more responsive to the needs of the SBML community. This page describes the plans for this *SBML Development Process*, and the current status of its implementation.

This SBML Development Process is being followed as of mid-2008.

The process described here evolved from previous proposals and discussions, and supercedes all previous SBML Development Process descriptions and proposals. (Previous proposals were presented at the following SBML Forum meetings: the **7th**, the **10th**, the **11th**, and the **12th**.) Some readers may recall that previous proposals involved additional components not described here (such as the formation of an "Architectural Board"); these ideas were dropped because of unenthusiastic community reception and the general goal of simplifying the SBML Development Process as much as possible.

Several other organizations served as sources of inspiration and ideas
 - Contents [hide]**
 - 1 Goals and Motivations for SBML
 - 2 Goals of the SBML Development Process
 - 3 SBML Community Organization
 - 3.1 The SBML Forum
 - 3.1.1 Requirements for membership
 - 3.1.2 Conduct of meetings
 - 3.2 The SBML Editors
 - 3.2.1 Responsibilities of SBML Editors
 - 3.2.2 Terms for SBML Editors
 - 3.2.3 Election process for SBML Editors
 - 3.2.4 Selection of the Chair of the SBML Editors
 - 3.3 The SBML Team
 - 4 SBML Development Procedures and Guidelines
 - 4.1 General Procedures and Guidelines
 - 4.1.1 Public participation
 - 4.1.2 Communication and transparency
 - 4.1.3 Achieving consensus
 - 4.2 Language Development Process
 - 4.2.1 SBML Levels, Versions, and Releases
 - 4.2.2 Process for SBML Level 2
 - 4.2.3 Process for SBML Level 3

Level 3 package	What it enables
Hierarchical composition	Models containing submodels
Flux balance constraints	Flux balance analysis models
Qualitative models	Petri net models, Boolean models
Spatial	Nonhomogeneous spatial models
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New table & status pages for package *specifications*

Documents/Specifications – SBML.org

<http://sbml.org/Documents/Specifications>

At this time, only *Version 1 Core* of SBML Level 3 has been released. Definitions of packages to go with Version 1 Core are expected in the very near future. When the specifications become available, they will be listed below. For now, you can find information about the ongoing activities in the [community wiki](#).

[edit] SBML Level 3 Version 1 Core

The most recent release of SBML Level 3 Version 1 Core is **Release 1**.

The Systems Biology Markup Language (SBML): Language Specification for Level 3 Version 1 Core

Authors: Michael Hucka, Frank Bergmann, Stefan Hoops, Sarah Keating, Sven Sahle, James Schaff, Lucian Smith, and Darren Wilkinson

This is the final Release 1 specification of 6 Oct. 2010.

The document link refers to the file on SourceForge.net. If you have any problems accessing the PDF file from there, a backup copy of the document is also available [locally from this server](#).

Specification →
Errata →
Submit issue →
Schemas →

Issues with the specification are tracked on the *issue tracker* whose link is indicated above. Accepted issues are periodically collected and listed on the *Errata* page indicated above. Once a general consensus emerges that the known errata warrant a new release of the SBML specification, a new *Release* is made.

[edit] SBML Level 3 Packages

Each individual SBML Level 3 package effort has an associated status page. Please follow the relevant links in the table below to find out more about a given package, including any draft specifications that may be available.

Package Name	Label	Description	Specification information page	Status
Arrays and Sets	arrays	Support for expressing arrays or sets of things	Arrays and Sets	
Annotations	annot	Support for richer annotation syntax than the regular annotations in SBML Level 3 Core	Annotations	
Hierarchical			Hierarchical	

New table & status pages for package *specifications*

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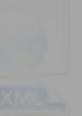
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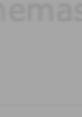
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Individual pages for package specification statuses

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- Address Bar:** Documents/Specifications/SBML Level 3/Packages/Hierarchical Model Composition (comp) – SBML.org
- Title Bar:** The Systems Biology Markup Language
- Header:** SBML.org, News, Documents (highlighted), Downloads, Forums, Facilities, Community, Events, About, E, RSS, G+, Google Site Search
- Breadcrumbs:** Parent pages: SBML.org / Documents / Specifications / SBML Level 3 / Packages
- Section Header:** Hierarchical Model Composition (comp)
- Section Subtitle:** SBML Level 3 Package Activity Status Page
- Table of Information:** A table listing package details:
 - Package name: Hierarchical Model Composition
 - Package label: comp
 - Package purpose: A means for defining how a model is composed from other models.
 - Package Working Group mailing list: [sbml-comp](#)
 - Contact address (where to ask questions): sbml-comp@lists.sourceforge.net
 - Specification status: Draft specification and/or implementations are in development.
 - Latest specification document: [Version of 30 July 2012](#)
 - Proposal status: Proposal approved.
 - Proposal document: [Proposal version of 18 May 2011](#)
 - Proposal activity page: [Proposal page for comp](#)
 - SBML Editor acting as liaison: [Lucian Smith](#)
- Note at bottom:** This table is generated automatically from the data for comp in the [SBML Level 3 Package Status spreadsheet](#).

New status tracking spreadsheet

SBML Level 3 Packages

<https://docs.google.com/spreadsheet/ccc?key=0ApbKgxVhXxVydG15WXIIT0JacHhwc0FPemV6bE1aQXc#gid=0>

File Edit View Insert Format Data Tools Help Insert Date Last edit was made 6 hours ago by mhucka

Label

1	A	B	C	D	E	G	H	J	L	
1	Label	Name	Description		Specification status	Link to specification information page	Link to current specification	Version/date of linked specification	Software Implementation status	Progress toward
2	annot	Annotations	Support for richer annotation syntax than the regular annotations in SBML Level 3 Core		Specification work has not started	http://sbml.org/Document	Not yet available	Not yet available	No applications are known to support this yet	Awaiting release of specification documents
3	arrays	Arrays and Sets	Support for expressing arrays or sets of things		Specification work has not started	http://sbml.org/Document	Not yet available	Not yet available	No applications are known to support this yet	Awaiting release of specification documents
4	comp	Hierarchical Model Composition	A means for defining how a model is composed from other models		Draft specification and/or implementations are in development	http://sbml.org/Document	http://sbml.org/images	30 July 2012	Implementations are known to be in development	Verifying the progress of draft specification software implementation
5	distrib	Distributions and Ranges	Support for expressing the idea that a given value is not known precisely but falls within some defined distribution or range		Specification work has not started	http://sbml.org/Document	Not yet available	Not yet available	No applications are known to support this yet	Awaiting release of specification documents
6	dyn	Dynamic Structures	Support for creating and destroying entities during a simulation		Specification work has not started	http://sbml.org/Document	Not yet available	Not yet available	No applications are known to support this yet	Awaiting release of specification documents
7	flux	Flux Balance Constraints	Support for constraint-based (a.k.a. steady-state) models		Draft specification and/or implementations are in development	http://sbml.org/Document	Not yet available	Not yet available	Implementations are known to be in development	Verifying the progress of draft specification software implementation
8	groups	Groups	A means for grouping elements		Specification work has not started	http://sbml.org/Document	Not yet available	Not yet available	No applications are known to support this yet	Awaiting release of specification documents
9	layout	Layout	Support for storing the spatial topology of a network diagram; adjunct to the render package		Draft specification and/or implementations are in development	http://sbml.org/Document	http://otto.bioquant.un	25 May 2011	Implementations are known to be in development	Verifying the progress of draft specification software implementation
10	multi	Multistate and Multicomponent Species	Object structures for representing entity pools with multiple states and composed of multiple components, and reaction rules involving them		Draft specification and/or implementations are in development	http://sbml.org/Document	http://sbml.org/Comm	14 April 2010	No applications are known to support this yet	Verifying the progress of draft specification software implementation
11	qual	Qualitative Models	Support for models wherein species do not represent quantity of matter & processes are not reactions per se		Draft specification and/or implementations are in development	http://sbml.org/Document	http://sbml.svn.sourceforge	5 November 2011	Two or more implementations have been released	Verifying the progress of draft specification software implementation
12	render	Rendering	Support for defining the graphical symbols and glyphs used in a diagram of the model; adjunct to the layout package		Draft specification and/or implementations are in development	http://sbml.org/Document	Not yet available	Not yet available	Implementations are known to be in development	Verifying the progress of draft specification software implementation
13	req	Required Elements	Support for fine-grained indication of SBML elements that have been changed by the presence of another		Specification work has not started	http://sbml.org/Document	Not yet available	Not yet available	Implementations are known to be in development	Awaiting release of specification documents

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<http://tinyurl.com/sbml-level-3-package-statuses>

Several package have made huge progress recently

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What is the SBML Test Suite?

System for testing SBML support in software

- Currently aimed at simulators (easiest to assess)
- Extensible architecture—easy to add more test cases

Components:

- Test models + simulation run parameters + expected results
 - Each case is labeled with tags that indicate tested features
- Online assessment system
- (Updated version forthcoming) Standalone test runner

Latest update

Version 2.1.0 contains **1123** test cases

- Note: tags have been revised—many cases have been retagged

Tested so far by

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<http://sf.net/projects/sbml/files/test-suite>

The Online SBML Test Suite

A screenshot of a web browser displaying the SBML.org main page. The browser interface includes a title bar with the text "Main Page - SBML.org" and a URL bar showing "sbml.org/Main_Page". The page itself has a blue header with the "SBML.org" logo and the text "The Systems Biology Markup Language". Below the header is a navigation menu with links for News, Documents, Downloads, Forums, Facilities, Community, Events, About, and social media icons for Twitter, RSS, and Google+. A search bar for "Google Site Search" is also present. The main content area features a welcome message about SBML, three sections for "For the curious", "For modelers", and "For software developers", and a sidebar for "SBML News" and "Community News" with recent updates.

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SBML would not have been possible without support from [multiple agencies and organizations](#), as well as intellectual contributions from many motivated

SBML News

SBML Test Suite updated (14 Aug. '12) Changes include new test cases, some tag updates and case corrections, and an updated online interface.

libSBML 5.6.0 released! (3 Aug. '12) libSBML 5.6.0 adds an R interface, improved Python interface, bug fixes, and more.

[Older news ...](#)

Community News

Antimony 2.3 beta (13 Aug. '12) Supports units, submodels, and the current SBML 'comp' draft specification.

BioModels Database rel. 23 (11 Aug. '12) The latest release adds new models and new services, esp. for the Path2Models project.

BioPAX2SBML 1.0 released (31 Jul. '12) BioPAX2SBML

The Online SBML Test Suite

A screenshot of a web browser displaying the SBML.org main page. A red speech bubble with the text "Find it here" points to the "Facilities" menu item, which is highlighted with a red circle. The page features the SBML.org logo, the title "The Systems Biology Markup Language", and three main sections: "For the curious", "For modelers", and "For software developers". On the right side, there are news feeds for "SBML News" and "Community News". At the bottom, there is a yellow button with the URL "http://sbml.org/Facilities/Online_SBML_Test_Suite".

Main Page - SBML.org

sbml.org/Main_Page

Find it here

SBML.org

The Systems Biology Markup Language

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Welcome to the portal for the Systems Biology Markup Language (SBML), a free and open interchange format for computer models of biological processes. SBML is useful for models of metabolism, cell signaling, and more. It continues to be evolved and expanded by an international community.

For the curious
What is SBML? Read our [introduction](#), then perhaps browse the [mailing lists](#) to glimpse what's happening with SBML today.

For modelers
Looking for software that supports SBML? Our [software guide](#) lists over 230 systems. Are you instead looking for models? Visit [BioModels Database](#), where you can find hundreds!

For software developers
Interested in supporting SBML in your software? Read our [basic introduction](#) and then the [SBML specifications](#) to understand how to use SBML. After that, you may want to look at [libSBML](#).

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outline

Brief summary of SBML for the unfamiliar

Recent development in Level 3 packages

Recent developments in the SBML Test Suite

Closing



Attendees at SBML 10th Anniversary Symposium, Edinburgh, 2010

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Japanese Ministry of Educ., Culture, Sports, Science and Tech.

BBSRC (UK)

National Science Foundation (USA)

DARPA IPTO Bio-SPICE Bio-Computation Program (USA)

Air Force Office of Scientific Research (USA)

STRI, University of Hertfordshire (UK)

Molecular Sciences Institute (USA)

I'd like your feedback!
You can use this anonymous form:

<http://tinyurl.com/mhuckafeedback>