

Updates about SBML

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(on behalf of many people)

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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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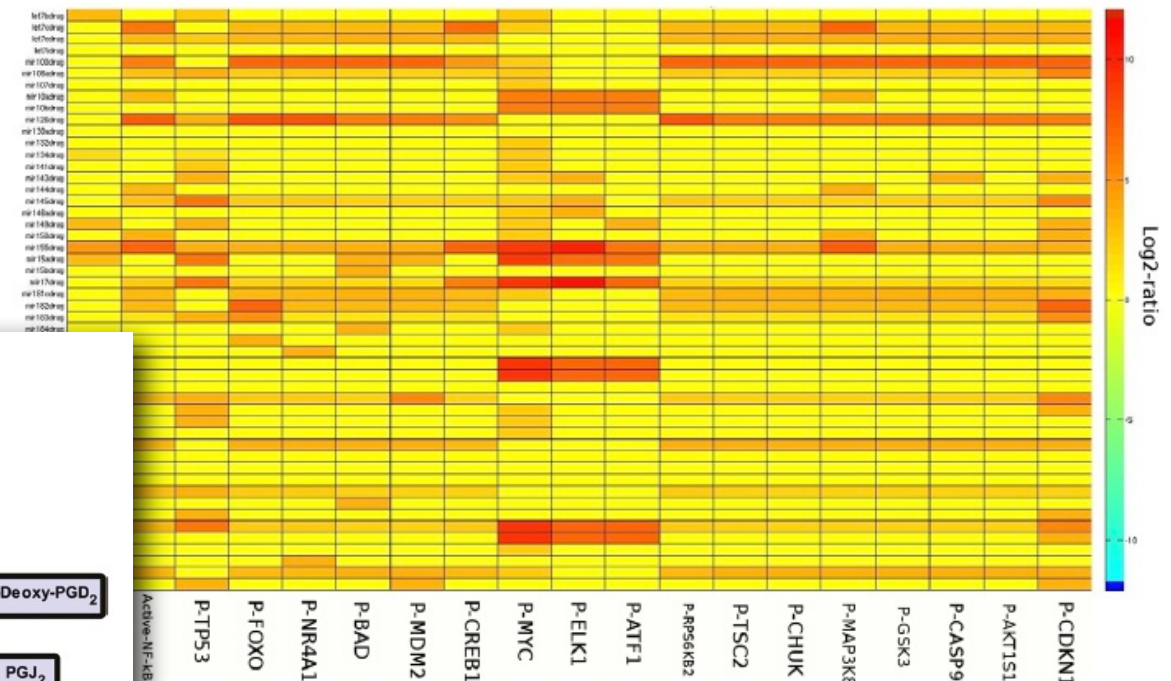
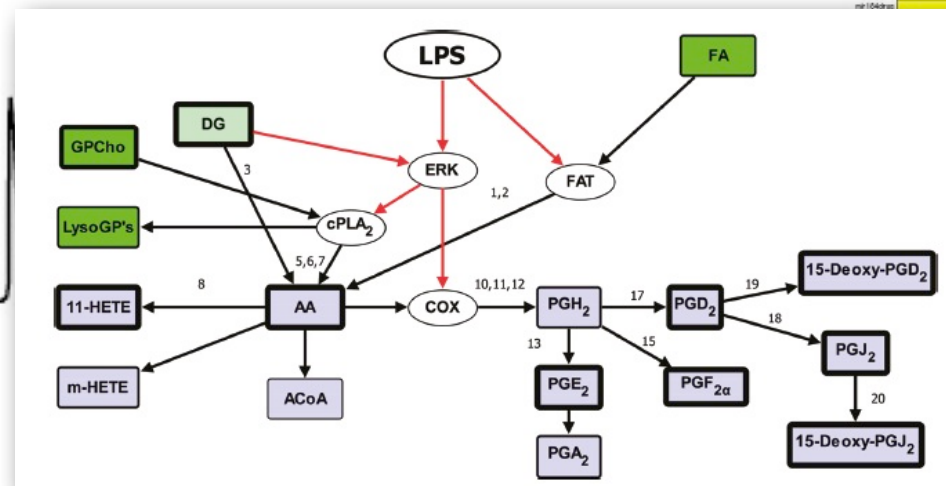
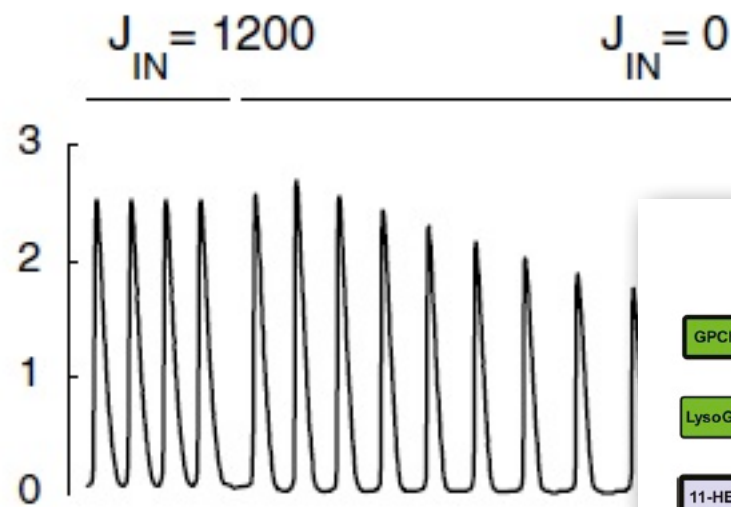
What are the outcomes of modeling and simulation?

Usually, there are at least two scientific outcomes:

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

Models come
in many forms

$$\begin{aligned}dx_1/dt &= -k_{12}[G]_{\text{out}}x_1 + k_{21}x_2 + k_{41}x_4 - k_{14}x_1, \\dx_2/dt &= k_{12}[G]_{\text{out}}x_1 - k_{21}x_2 - k_{23}x_2 + k_{32}x_3, \\dx_3/dt &= k_{23}x_2 - k_{32}x_3 - k_{34}x_3 + k_{43}[G]_{\text{in}}x_4, \\dx_4/dt &= k_{34}x_3 - k_{43}[G]_{\text{in}}x_4 - k_{41}x_4 + k_{14}x_1.\end{aligned}$$



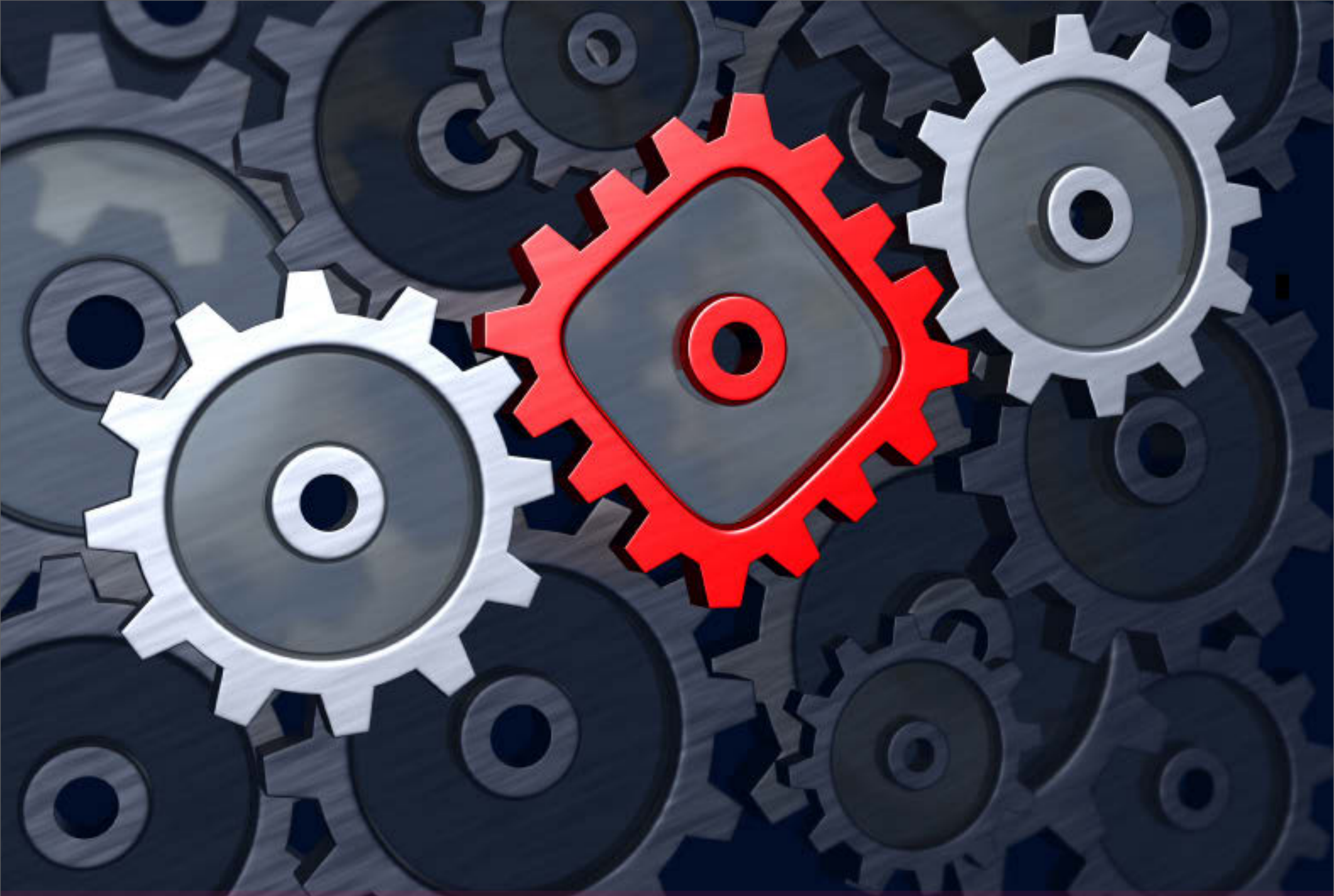
Models a fundamentally important scientific work product

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—

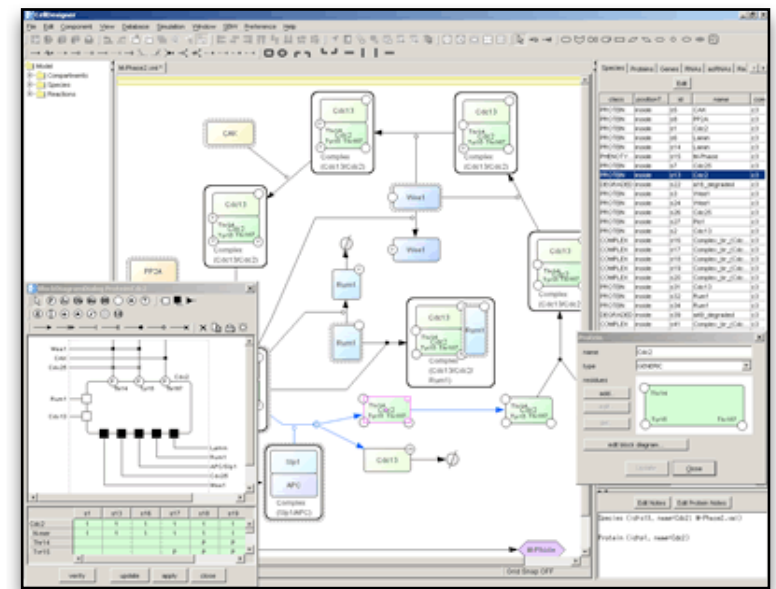
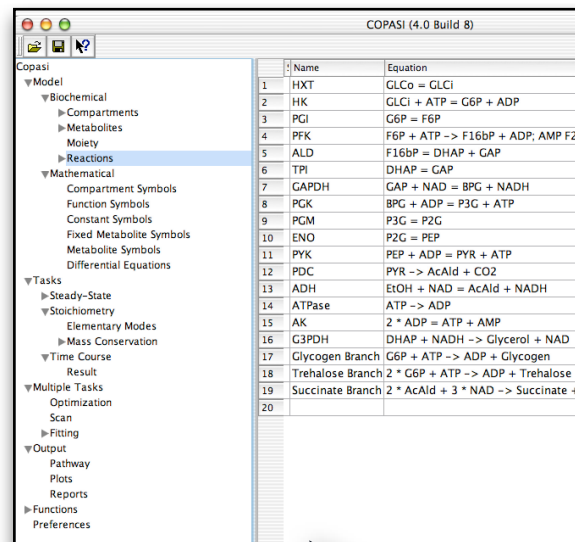
- **Reduce ambiguity** in communication
- Offer a **concrete framework** for adding new data and theories
- **Support direct evaluation** of relationships between theories



Different tools \Rightarrow different representation languages

Communication is better with interoperable data formats

SBML: a lingua franca for software



EMBL-EBI BioModels Database

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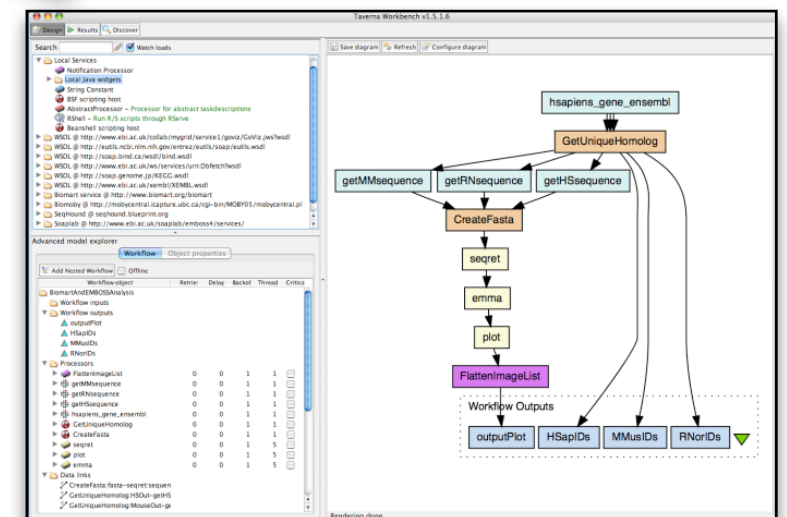
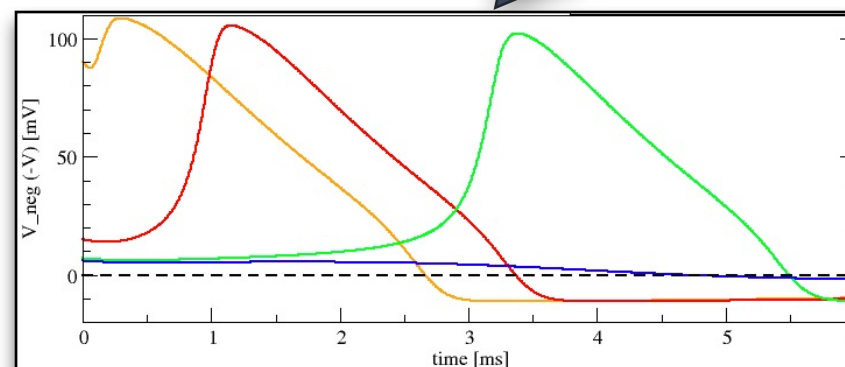
Databases Tools Research Training Industry About Us

BioModels Home Models Submit Support About BioModels

BioModels Database - A Database of Annotated Published Models

BioModels Database is a repository of peer-reviewed, published, computational models. These mathematical models are primarily from the field of systems biology, but more generally are those of biological interest. This resource allows biologists to store, search and retrieve published mathematical models. In addition, models in the database can be used to generate sub-models, can be simulated online, and can be converted between different representational formats. This resource also features programmatic access via Web Services.

All unmodified models in the database are available freely for use and distribution, to all users. This resource is developed and maintained by the [BioModels.net](http://www.biomodels.net) initiative. More information about BioModels Database can be found in the [Frequently Asked Questions](#).



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**)

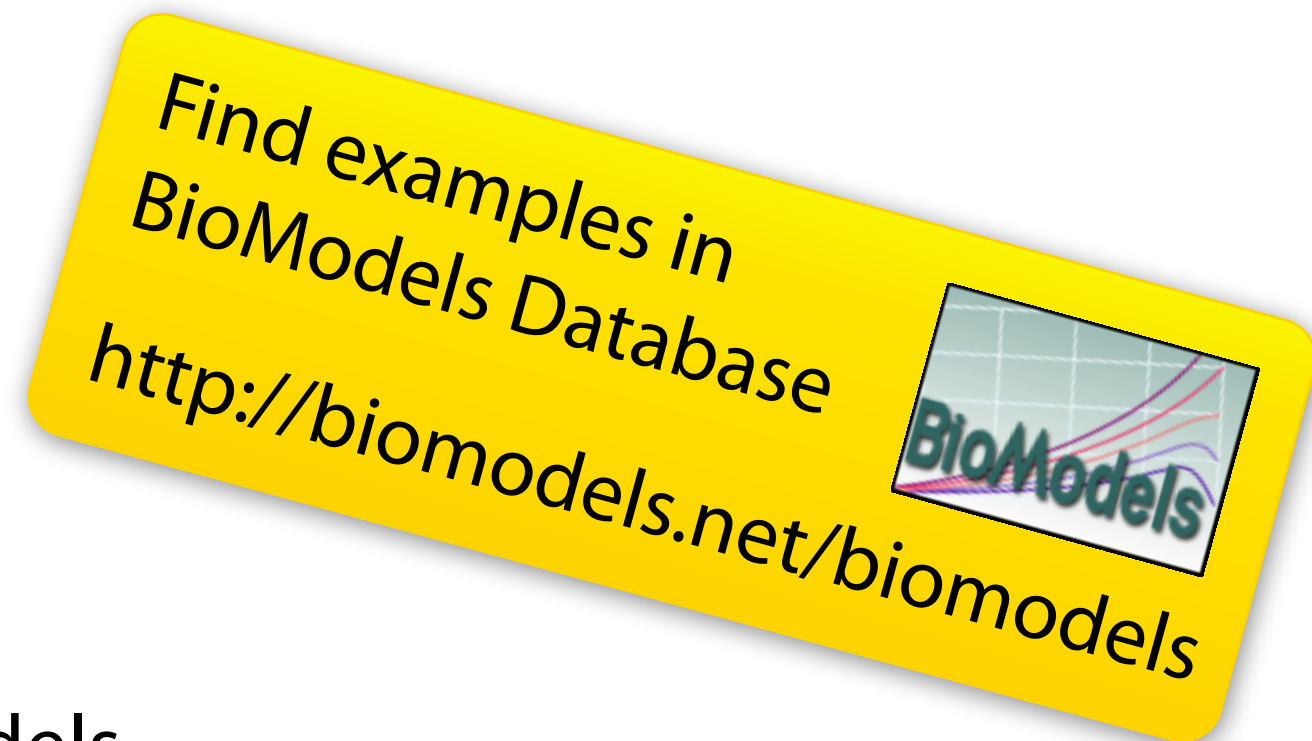
Models can further include:

- 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



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

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The Systems Biology Markup Language

News Documents Downloads Forums Facilities Community Events About

Google Site Search...

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.

MatCont 4.1 supports SBML
(29 Jun. '11) [MatCont](#) is a MATLAB package for studying parameterized continuous and discrete dynamical systems.

iPathways 1.1 released
(15 Jun. '11) [iPathways](#) is

Find software in the SBML Software Guide

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Main Page - SBML.org

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SBML.org The Systems Biology Markup Language

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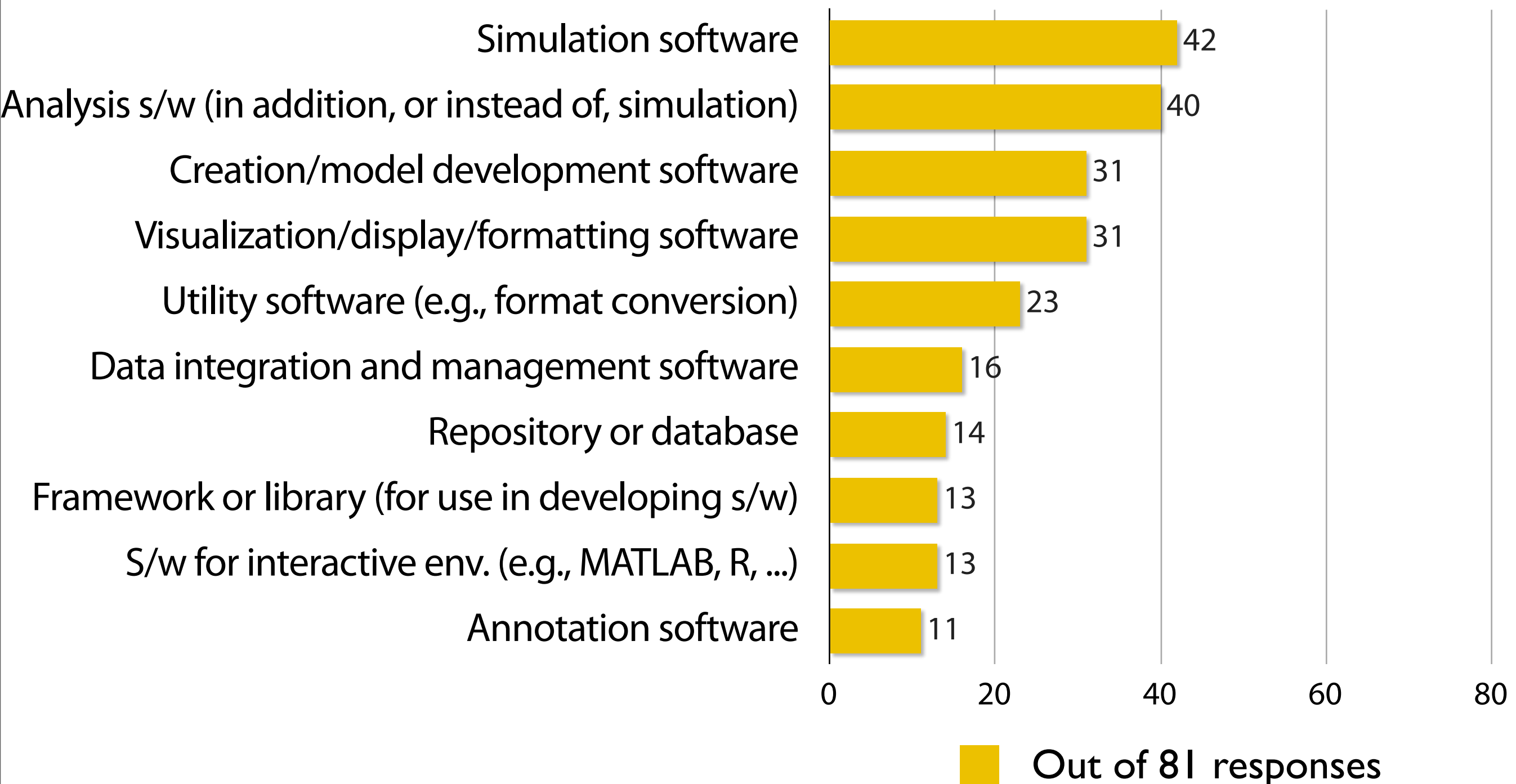
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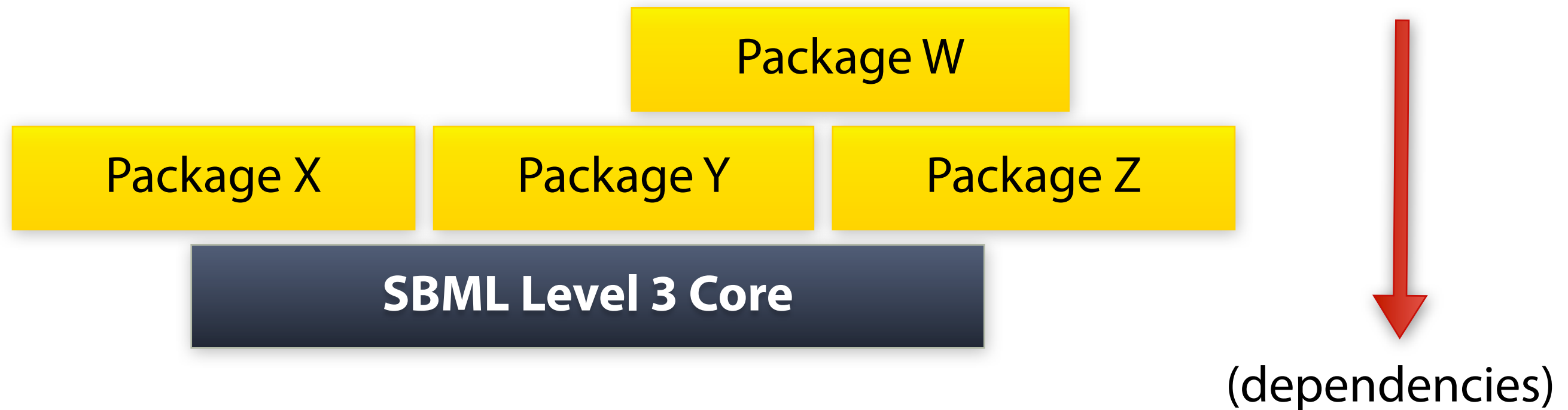
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Results of 2011 survey of SBML-compatible software

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 address bar displaying `http://sbml.org/Documents/SBML_Development_Process`. The browser's address bar also shows the page title "Documents/SBML Development Process - SBML.org". The browser's toolbar includes a "Reader" button and a "Word" button. The browser's status bar shows a list of tabs: "1 pkt", "2 wos", "3 tom", "4 saf", "5 pt", "6 jrs", "7 sc", "8 spr", "9 g", "tools", "\$\$", "search", "sys", "data", "web", "code".

The website's header features the SBML.org logo on the left and the text "The Systems Biology Markup Language" on the right. Below the header is a navigation bar with links: "News", "Documents", "Downloads", "Forums", "Facilities", "Community", "Events", "About", and a "Google Site Search" box. The "Documents" link is highlighted.

The main content area has a breadcrumb trail: "Parent pages: SBML.org / Documents". The title "SBML Development Process" is displayed in a large, bold font. The text below the title describes the development process, mentioning the adoption of a participative, community-oriented approach in the early years of SBML, and the need for a more formal organization and systematic process starting in 2003. It also mentions that the process is being followed as of mid-2008.

On the right side of the page, there is a "Contents [hide]" section with a list of links to various parts of the document:

- 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
Multicomponent species	Entities with structure & state; rule-based models
Graph layout	Diagrams of models
Graph rendering	Diagrams of models
Distribution & ranges	Nonscalar values
Annotations	Richer annotation syntax
Groups	Arbitrary grouping of model components
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New table & status pages for package *specifications*

Documents/Specifications - SBML.org

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

SBML

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 →



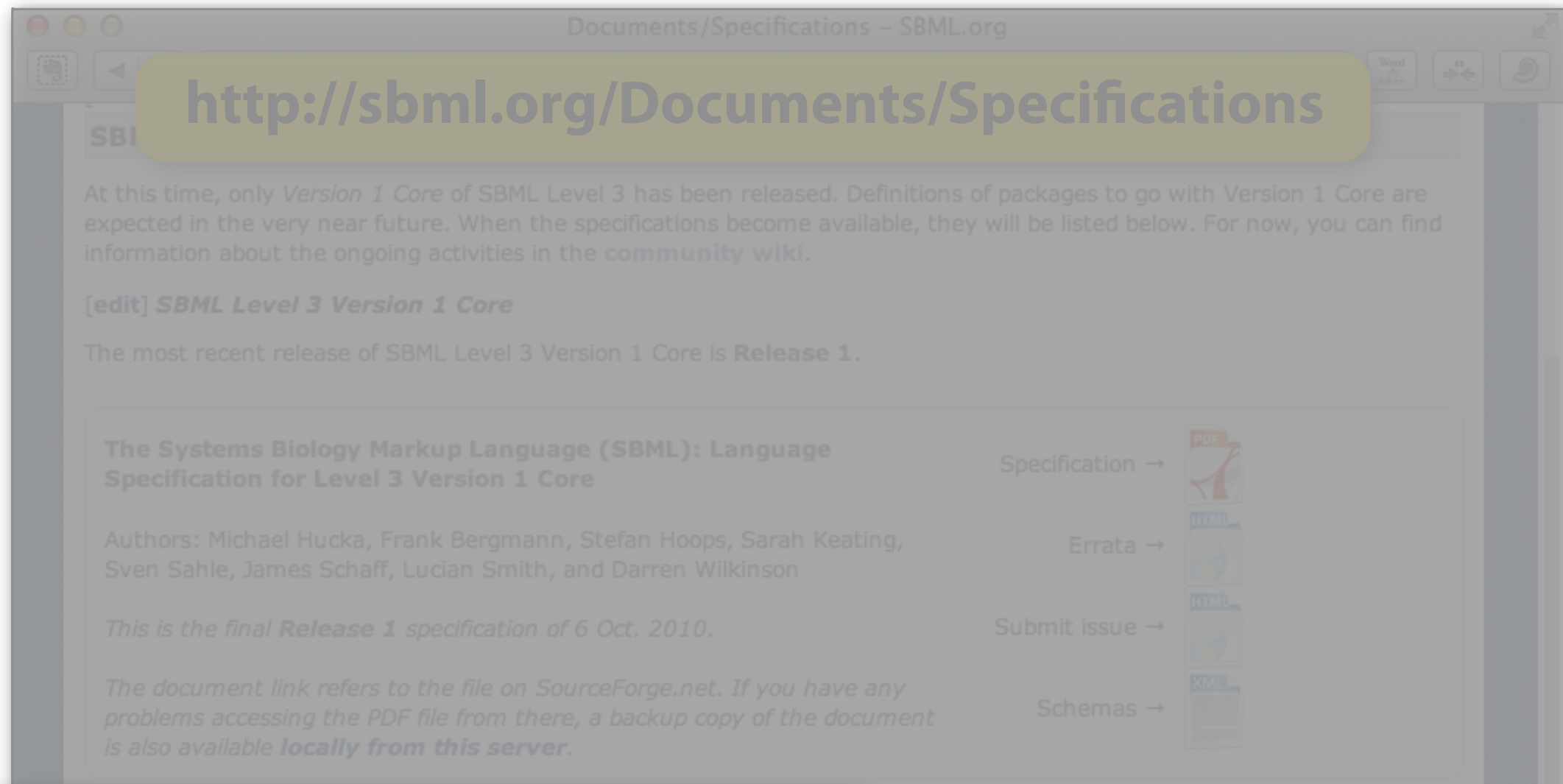
Issues with the specification are tracked on the *issue tracker* whose link is indicated above. Accepted issues are periodically collected and listed on the *Errata* page indicated above. Once a general consensus emerges that the known errata warrant a new release of the SBML specification, a new *Release*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



New table for package specifications

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Individual pages for package specification statuses

Documents/Specifications/SBML Level 3/Packages/Hierarchical Model Composition (comp) - SBML.org

http://sbml.org/Documents/Specifications/SBML_Level_3/Packages/Hierarchical_Model_Con

SBML.org The Systems Biology Markup Language

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Parent pages: [SBML.org](#) / [Documents](#) / [Specifications](#) / [SBML Level 3](#) / [Packages](#)

Hierarchical Model Composition (comp)

SBML Level 3 Package Activity Status Page

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 liason:	Lucian Smith

This table is generated automatically from the data for comp in the [SBML Level 3 Package Status](#) spreadsheet.

SBML Level 3 Package Activity Status Page

New status tracking spreadsheet

SBML Level 3 Packages

https://docs.google.com/spreadsheet/ccc?key=0ApbKgxVhXxVydG15WXlIT0JacHhwc0FPemV6bE1aQXc#gid=0

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fx | Label

	A	B	C	D	E	G	H	J	L	
	Label	Name	Description		Specification status	Link to specification information page	Link to current specification	Version/date of linked specification	Software Implementation status	Progress towards specification
1										
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 draft
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 draft
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 implementations
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 draft
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 draft
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 implementations
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 draft
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 implementations
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 implementations
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.source	5 November 2011	Two or more implementations have been released	Verifying the progress of draft specification; software implementations
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 implementations
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 draft

New status tracking spreadsheet

SBML Level 3 Packages

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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

- iBioSim (Chris Myers)
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New cases developed by Lucian Smith using Antimony

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The Online SBML Test Suite

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For modelers
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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

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



The screenshot shows the SBML.org website. A red callout bubble with the text "Find it here" points to the "Facilities" link in the navigation bar. The website header includes the SBML.org logo and the title "The Systems Biology Markup Language". The navigation bar contains links for News, Documents, Downloads, Forums, Facilities, Community, Events, and About. A Google Site Search bar is also present. The main content area features a welcome message and three sections: "For the curious", "For modelers", and "For software developers". The right sidebar contains "SBML News" and "Community News" sections.

Find it here

SBML.org The Systems Biology Markup Language

News Documents Downloads Forums **Facilities** Community Events About

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.

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http://sbml.org/Facilities/Online_SBML_Test_Suite

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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Keio University (Japan)

International Joint Research Program of NEDO (Japan)

Japanese Ministry of Agriculture

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>