Update on SBML

Michael Hucka, Ph.D.

Department of Computing + Mathematical Sciences
California Institute of Technology
Pasadena, CA, USA

Email: mhucka@caltech.edu *Twitter: @mhucka*

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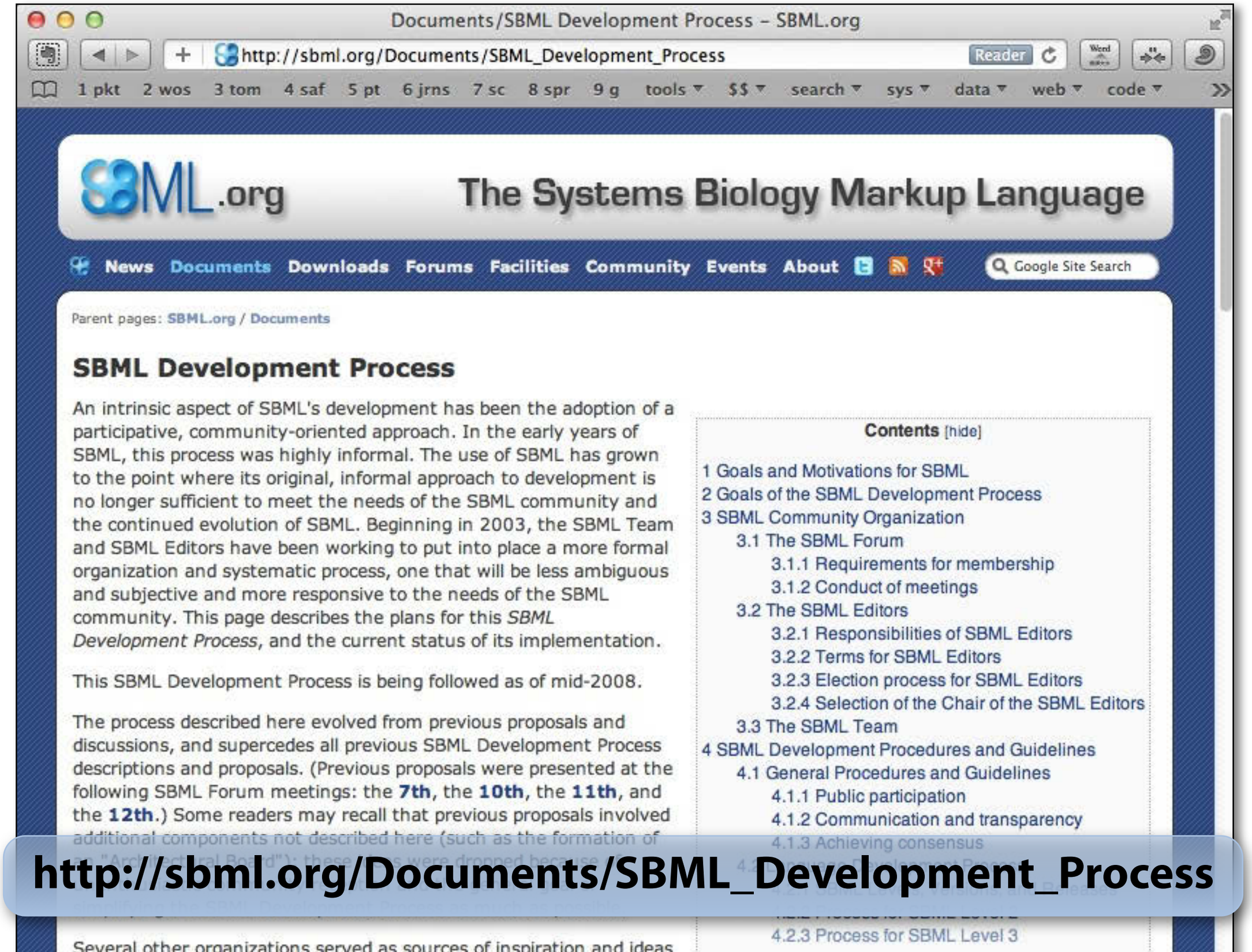
SBML Development Process



http://sbml.org/Documents/SBML_Development_Process

The SBML Editors

(*Chair*) Michael Hucka (Ph.D. in Computer Science and Engineering) is a Member of the Professional Staff at **Caltech**. He has Chaired the SBML Editors and SBML Team since 2003. He works on all aspects of SBML and is involved with **BioModels.net** consortium efforts such as **BioModels Database**.

Frank Bergmann (Ph.D. in Computation & Systems Biology) is a Research Fellow in the **department for modeling of biological processes at the University of Heidelberg** and a member of the SBML Team. He is the lead software developer for the **Systems Biology Workbench** and is also one of the programmers on **COPASI**.

Sarah Keating (Ph.D. in Electronic & Electrical Engineering) is a Senior Software Developer at the **EBI**, working remotely for the SBML project. She works as part of the SBML Team on developing software infrastructure for the support of the SBML standard.

Nicolas Le Novère (Ph.D. in Molecular Pharmacology) is

Chris J. Myers (Ph.D. in Electrical Engineering) is a

Sven Sahle (Ph. D. in Theoretical Chemistry) is a junior group

Towards Version 2 of SBML Level 3 and Version 5 of Level 2

Have been collecting issues – some small, some significant

- SourceForge tracker

  http://sourceforge.net/p/sbml/sbml-specifications/

- SBML Editor discussions

  http://sbml.org/Events/SBML_Editors%27_Meetings

Goal (for this COMBINE): settle changes

- Focus on what *needs* to be done
  - Editors are conscious of impact on backward compatibility

Detailed 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**	

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New table for package specifications

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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	
1	**Label**	**Name**	**Description**		**Specification status**	**Link to specification information page**	**Link to current specification**	**Version/date of linked specification**	**Software implementation status**	**Progress tow**
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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 relea specification d
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 relea specification d
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 p draft specificat software imple
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 relea specification d
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 p draft specificat software imple
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 p draft specificat software imple
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 p draft specificat software imple
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http://tinyurl.com/sbml-level-3-package-statuses

Level 3 package	What it enables	Status
Hierarchical model composition	Models containing submodels	✔
Flux balance constraints	Constraint-based models	✔
Qualitative models	Petri net models, Boolean models	✔
Graph layout	Diagrams of models	✔
Multicomponent/state species	Entities w/ structure; also rule-based models	draft
Spatial	Nonhomogeneous spatial models	draft
Graph rendering	Diagrams of models	draft
Groups	Arbitrary grouping of components	draft
Distributions	Numerical values as statistical distributions	in dev
Arrays & sets	Arrays or sets of entities	in dev
Dynamic structures	Creation & destruction of components	in dev
Annotations	Richer annotation syntax	

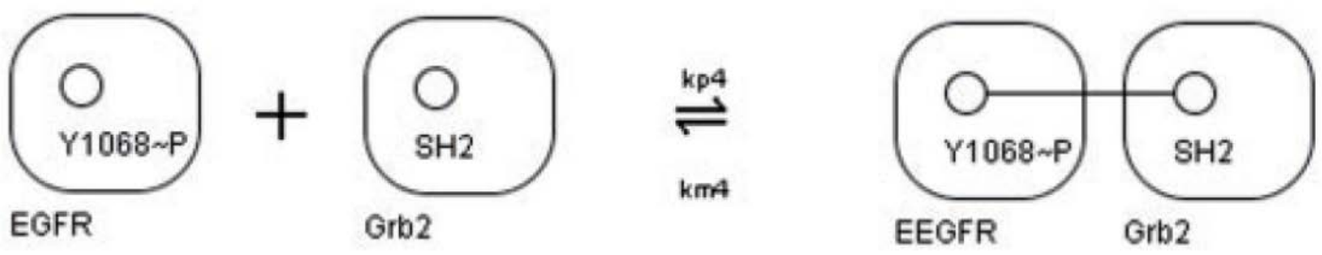
Multistate, Multicomponent and Multicompartment species

Core SBML lacks support for structured entities and pattern rules

- Different states of molecular entities must be different entities/species

SBML Level 3 effort for "multi" aims to add support for structures & patterns

- First proposals were by Finney, Blinov, Faeder, Hlavacek, Le Novère
- Revived by F. Zhang from Simmune group (Meier-Schellersheim et al.)
- Aspects of new effort: species types, binding sites, complexes, rules



Active discussions on "sbml-multi" mailing list – more info:

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

SBML Level 3 Spatial models (draft)

Main components:

- Definition of **coordinate systems**
- Definition of patches of **spatial geometries**, called domains
  - A domain is a contiguous patch of volumetric space or a contiguous surface patch
- **Mapping** of SBML compartments, species, & parameters to domains
- Definition of new **molecular transport mechanisms** (advection, diffusion, boundary conditions)
- **Mapping** of molecular transport mechanisms to domains

Draft developed & implemented by Jim Schaff of the Virtual Cell group

- Beta implementation for libSBML available today

Lucian Smith has lately been working on the specification

SBML Level 3 Distributions

Goal: allow statistical distributions of values

Status: close to convergence?