

SBML Team facilities & software

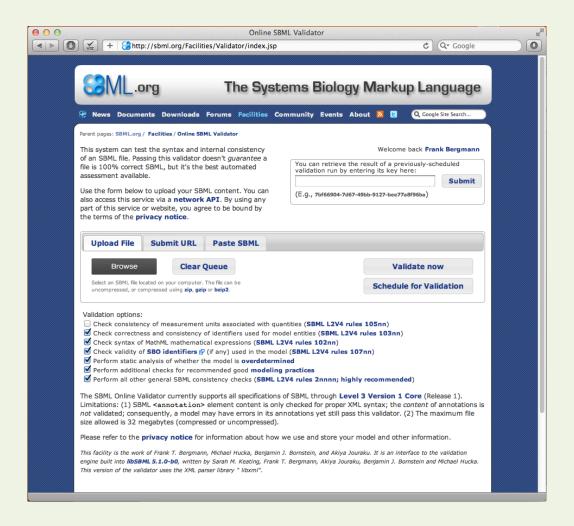
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Sarah Keating

On behalf of the SBML Team

ONLINE VALIDATOR

http://sbml.org/Facilities/Validator



Options for Direct or Scheduled Validation

Direct Validation

- Intended for (smallish)
 models, or inexpensive
 validation runs (i.e., not for
 unit validation on models
 with thousands of
 reactions)
- 60 second timeout
- Yields results directly

Scheduled Validation

- Intended for all cases where validation is expected to take longer
- After scheduling you will receive a validation identifier that you can use later to retrieve the results
- Results will be kept for 24 hours

Customizable Error List



Error Categories

Units consistency

Category of errors that can occur while validating the units of measurement on quantities in a model.

ErrorId	Meaning	L1V1	L1V2	L2V1	L2V2	L2V3	L2V4	L3V1
10501	Units of arguments to function call do not match function's definition	Warning	Warning	Warning	Error	Error	Warning	Warning
10503	Inconsistent <kineticlaw> units</kineticlaw>	N/A	N/A	N/A	N/A	N/A	N/A	Warning
10511	Mismatched units in assignment rule for compartment	Error	Error	Error	Error	Error	Warning	Warning
10512	Mismatched units in assignment rule for species	Error	Error	Error	Error	Error	Warning	Warning
10513	Mismatched units in assignment rule for parameter	Error	Error	Error	Error	Error	Warning	Warning
10514	Mismatched units in assignment rule for stoichiometry	N/A	N/A	N/A	N/A	N/A	N/A	Warning
10521	Mismatched units in initial assignment to compartment	N/A	N/A	N/A	Error	Error	Warning	Warning
10522	Mismatched units in initial assignment to species	N/A	N/A	N/A	Error	Error	Warning	Warning
10523	Mismatched units in initial assignment to parameter	N/A	N/A	N/A	Error	Error	Warning	Warning
10524	Mismatched units in initial assignment to stoichiometry	N/A	N/A	N/A	N/A	N/A	N/A	Warning
10531	Mismatched units in rate rule for compartment	Error	Error	Error	Error	Error	Warning	Warning
10532	Mismatched units in rate rule for species	Error	Error	Error	Error	Error	Warning	Warning
10533	Mismatched units in rate rule for parameter	Error	Error	Error	Error	Error	Warning	Warning
10501	Mismatched units in rate rule for			B1 / B	B1 / B		B1 / B	

 Invoke the validator by POST ing a file to it, or passing in a URL (with an API Key)

```
curl -F file=@filename.xml
  -F output=text
  -F offcheck=u,p,s
  http://sbml.org/validator/
```

 Invoke the validator by POST ing a file to it, or passing in a URL (with an API Key)

```
curl -F url=<URL>
    -F apikey=<KEY>
    -F output=text
    -F offcheck=u,p,s
    http://sbml.org/validator/
```

```
    Invoke the validator by POST ing a file to it or

$ curl -F url=http://sbml.org/validator/api/sample-02.xml
File: sample-02.xml
Options:
  Units consistency checking: off
  Identifier consistency checking: on
  MathML consistency checking: on
  SBO consistency checking: on
  Overdetermined model checking: on
  Modeling practices checking: on
  Overall SBML consistency checking: on
Results: The web request could not be authenticated.
```

nttp://spmi.org/validator/

User information

Name: Frank Bergmann

Email Address: fbergman@caltech.edu

API Key: 1f234c22-7162-43e3-8715-3a10686dc33c

Software (optional): SBML Validator

Log out

Change Password



Get new key

Web Service

```
String convertSBML(String sbmlModel,
                   int targetLevel, int targetVersion)
String convertSBMLtoHTML(String content)
String expandFunctionDefinitions(String sbmlModel)
String expandInitialAssignments(String sbmlModel)
String getLibSBMLVersion()
String validateSBML(String sbmlModel, boolean withUnits,
             boolean withIdentifiers, boolean withMathML,
             boolean withSBO, boolean withOverdetermined,
             boolean withModelingPractices, boolean withGeneral)
String validateSBMLBuffer(byte[] sbmlContent, String type,
boolean withUnits, boolean withIdentifiers, boolean withMathML,
boolean withSBO, boolean withOverdetermined, boolean
withModelingPractices, boolean withGeneral)
String validateSBMLBufferWithoutUnitChecks(byte[] sbmlContent,
String type)
String validateSBMLWithoutUnitChecks(String sbmlModel)
```

SOFTWARE INDEX

SBML Software Tools Survey

eneral information about your	software	
eneral information about your	Sortware	
1/6		
•	nay also use	the information to write papers about SBML
What is your name ? (This is to verify the enter in this form; your name will not be		What is your email address ? (Again, this is to verify the information you enter; your name will not be put in the Guide.)
software. What is your name? (This is to verify the enter in this form; your name will not be SBML Software Guide.)		is to verify the information you enter; your

Updated: Software Matrix

SBML Software Matrix

This matrix provides an at-a-glance summary of software known to us to provide some degree of support for reading, writing, or otherwise working with SBML. The columns' meanings are explained below. For a list of longer descriptions grouped into themes, please see our **SBML Software Summary** page. Please use the **survey form** to notify us about omissions, updates and suggestions.

			Сар	abil	ities	5	Frameworks							API	Dep.		Platforms				ML	Availabil.			
	Recent contact	Creation	Simulation	Analysis	Database	Utility	90E	DAE	PDE	Stochastic	Events	Logical	Other			Linux	Mac OS X	Windows	Web Browser	Import	Export	Open source	Academic use	Commercial use	
ABC-SysBio				•			•			•					Python	•	•	•		•		•	F	F	1
acslXtreme		•																•		•			\$	\$	ľ
ALC		•					•	•		•			•			•	•	•	•		•	•	F	F	
Antimony	•	•				•								C, C++		•	•	•		•	•	•	F	F	
Arcadia	•					•	•	•	•	•	•	•	•			•	•	•							
Asmparts		•				•	•									•		•		•	•	•	F	F	
Athena	•	•	•	•	•	•	•			•	•	•	•	SBW, .NET				•		•	•	•	F	F	
AutoSBW	•			•			•							SBW	SBW	•		•		•	•	•	F	F	
AVIS													•			•				•		•	F	F	
BALSA		•													Sigtran										
BASIS	•	•	•		•		•			•	•			Web Services					•	•	•	•	F	F	
BetaWB	•	•	•	•						•	•					•	•	•			•		F	F	
Bifurcation Discovery Tool				•			•								SBW	•	•					•	F	F	
BiGG					•														•		•		F		
BiNoM	•	•		•		•							•			•	•	•		•	•	•	F	F	
BiNoM Cytoscape Plugin															Cytoscape								F	F	
This matrix was general									<u>.</u>						DisChanne								F	F	

Updated: Software Summary

SBML Software Summary

This page lists software known to us to provide some degree of support for reading, writing, or otherwise working with SBML. For an at-a-glance matrix summarizing key features of these software packages, please see our SBML Software Matrix page. Please use the survey form & to notify us about additions and suggestions.

Note that several of the ODE/DAE-based simulators also include some form of stochastic simulation capability, and viceversa. Also most of the model simulation, development, and analysis tools listed elsewhere on this page include some form of visualization.

Analysis software

- ABC-SysBio ABC-SysBio implements likelihood free parameter inference and model selection in dynamical systems. It is designed to work with both stochastic and deterministic models written in Systems Biology Markup Language (SBML). ABC-SysBio is a Python package that combines three algorithms: ABC rejection sampler, ABC SMC for parameter inference and ABC SMC for model selection.
- AutoSBW ☑ A frontend around AUTO to simplify bifurcation analysis.
- Bifurcation Discovery Tool
 — The Bifurcation Discovery Tool uses a
 genetic algorithm to search for Hopf bifurcations, turning points, and
 bistable switches. The user can select parameters to be searched,
 admissible parameter ranges, and the nature of the bifurcation to be
 sought. The tool returns parameter values for the model for which the
 particular behavior is observed.

Contents [hide]

- 1 Analysis software
- 2 Annotation software
- 3 Creation/development software
- 4 Data integration and management software
- 5 Framework or library
- 6 Repository or database
- 7 Scripting module
- 8 Simulation software
- 9 Utility software
- 10 Visualization software

New: Software Showcase

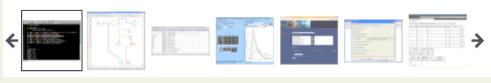
SBML Software Showcase

The following slideshow of SBML-compatible software systems contains the subset of packages for which we were provided screenshots by the software's authors. For a complete listing of SBML software, see the SBML Software Matrix, and for a list of longer descriptions grouped into themes, please see our SBML Software Summary page.

JarnacLite

JarnacLite allows to edit SBML through a simple script based format. It is integrated with SBW, so that a model created with JarnacLite can be quickly simulated and analyzed with a variety of tools. JarnacLite is available on all platforms, and as translator also online. It is released under the BSD license.

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In Development: Software Index



SBML TOOLBOX 4.0.1

SBMLToolbox 4.0.1

Home / SBMLToolbox / 4.0.1 Name * Parent folder README.txt SBMLToolbox-4.0.1.zip Totals: 2 Items S B M L Toolbox 4.0.1

SBMLToolbox 4.0.1

- import and export removed to libSBML
- improved simulation (passes 450 tests from SBML Test-suite)
- improved creation of SBML models
- removed GUI support (fully octave compatible)
- improved documentation

SBMLToolbox 4.0.1

SBMLToolbox 4.0 API Manual

SBMLToolbox 4.0 API

This manual describes the application programming interface (API) of SBMLToolbox, an open-source (LGPL) MATLAB/Octave toolbox for writing and manipulating content in the Systems Biology Markup Language (SBML). This version of SBMLToolbox supports all releases of SBML up through Level 3 Version 1 Core Release 1. For more information about SBML, please visit http://sbml.org on the Internet.

All functions can be used in both the MATLAB and Octave environments.

Installation

• Installation

Functions

- Accessing the model
- Convenience functions
- Simulation functions
- Validation functions

MATLAB_SBML Structure Functions

- General functions
- Fieldname functions
- AlgebraicRule
- AssignmentRule
- Compartment
- CompartmentType
- CompartmentVolumeRule
- Constraint
- Delay
- EventAssignment
- FunctionDefinition
- InitialAssignment
- KineticLaw
- KineticLaw
 LocalParameter
- Model
- ModifierSpeciesReference
 Parameter

SBMLToolbox 4.0 API Manual

ACCESSMODEL

The AccessModel folder contains a number of functions that derive information from the MATLAB_SBML structures.

Function are:

array = DetermineSpeciesRoleInReaction(SBMLSpecies, SBMLReaction)

Takes

- 1. SBMLSpecies, an SBML species structure
- 2. SBMLReaction, an SBML reaction structure

Returns

 an array with five elements [isProduct, isReactant, isModifier, positionInProductList, positionInReactantList] indicating whether the species is a product, reactant or modifier and re position in the list of products/reactants

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1. array = 0 if the species is NOT part of the reaction

EXAMPLE:

111	У	-	Det	erm	ine	Spe	cies	Role:	[n]	Rea	ction(s, r)
	-	=	0								not in r
		=	[1,	٥,	٥,	2,	0]	if	3	is	product number 2 in rb
		=	[0,	1,	٥,	٥,	1]	if	3	is	reactant number 1 in r
		=	[0,	Ο,	1,	Ο,	0]	if	3	is	a modifier in r
		=	[1,	1,	Ο,	1,	2]	if	3	is	product number 1 and reactant number

[names, values] = GetAllParameters(SBMLModel)

Takes

1. SBMLModel, an SBML Model structure

Returns

- 1. an array of strings representing the identifiers of all parameters (both global and embedded) within
- 2. an array of the values of each parameter

NOTE: the value returned will be (in order)

- · determined from assignmentRules/initialAssignments where appropriate
- . the attribute 'value' for the given parameter
- NaN, if the value is not specified in any way within the model

SBMLToolbox 4.0 API Manual

2

Model

typecode = SBML MODEL

SBML Level 1

Version	n 1	Version 2				
Fieldname	Туре	Fieldname	Туре			
typecode	as above	typecode	as above			
notes	string	notes	string			
annotation	string	annotation	string			
SBML_level	double	SBML_level	double			
SBML_version	double	SBML_version	double			
name	string	name	string			
unitDefinition	array of structures	unitDefinition	array of structures			
compartment	array of structures	compartment	array of structures			
species	array of structures	species	array of structures			
parameter	array of structures	parameter	array of structures			
rule	array of structures	rule	array of structures			
reaction	array of structures	reaction	array of structures			

SBML Level 2

Version	n 1	Version 2					
Fieldname	Туре	Fieldname	Туре				
typecode	as above	typecode	as abo				
metaid	string	metaid	string				
notes	string	notes	string				
annotation	string	annotation	string				

http://sbml.org/Software/SBMLToolbox/SBMLToolbox_4.0_API_Manual

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