SBML Team facilities & software
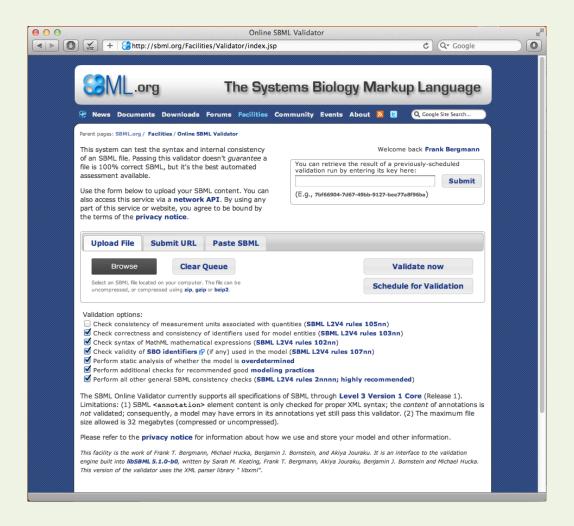
Frank T. Bergmann

Sarah Keating

On behalf of the SBML Team

ONLINE VALIDATOR

http://sbml.org/Facilities/Validator
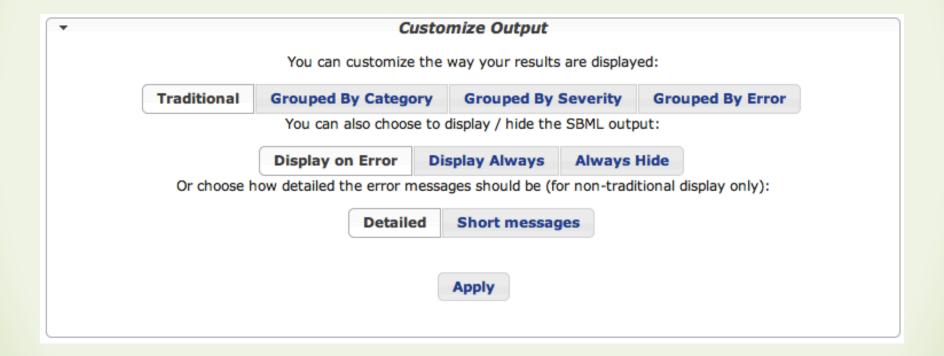
Options for Direct or Scheduled Validation

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	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
10534	Mismatched units in rate rule for	N/A	N/A	N/A	N/A	N/A	N/A	Warning

REST API

- 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/
```

http://sbml.org/Facilities/Documentation/Validator_Web_API

REST API

- 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/
```

REST API

- 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.
```

http://sbml.org/validator/

REST API

User information

Name: Frank Bergmann

Email Address: fbergman@caltech.edu

API Key: 1f234c22-7162-43e3-8715-3a10686dc33c   **Get new key**

Software (optional): SBML Validator

Log out   **Change Password**

◀ Return to the SBML Validator front page.

http://sbml.org/Facilities/Documentation/Validator_Web_API

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)
```

http://sbml-validator.caltech.edu:8888/validator_ws/services/LibSBML?wsdl

SOFTWARE INDEX

SBML Software Tools Survey

Parent pages: **SBML.org** / **SBML Software Guide**

SBML Software Details Questionnaire

General information about your software

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Please fill out this form to tell us about your SBML-compatible software. We will use this information to update the **SBML Software Guide**. We may also use the information to write **papers about SBML software**.

What is **your name**? (This is to verify the info you enter in this form; your name will not be put in the SBML Software Guide.)

What is **your email address**? (Again, this is to verify the information you enter; your name will not be put in the Guide.)

What is the public **contact address** for the software? Generally this is an email address (possibly the same as the one above, if you wish), although it can be an online help form instead.

What is the URL to the **home page of your software**?

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.

	Recent contact	Capabilities					Frameworks							API	Dep.	Platforms				SBML		Availabil.		
		Creation	Simulation	Analysis	Database	Utility	ODE	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
acslXtreme		•																•		•			$	$
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
Bio-Sketch Pad		•													BioChara								F	F

This matrix was generated on 2011-07-19 (total number of tools: 230)

http://sbml.org/SBML_Software_Guide/SBML_Software_Matrix

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 vice-versa. 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]

http://sbml.org/SBML_Software_Guide/SBML_Software_Summary

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New: Software Showcase

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
- Event
- EventAssignment
- FunctionDefinition
- InitialAssignment
- 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

1. 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

or

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

EXAMPLE:

```
y   =   DetermineSpeciesRoleInReaction(s, r)
    =   0                 if s is not in r
    =   [1, 0, 0, 2, 0]   if s is product number 2 in rb
    =   [0, 1, 0, 0, 1]   if s is reactant number 1 in r
    =   [0, 0, 1, 0, 0]   if s is a modifier in r
    =   [1, 1, 0, 1, 2]   if s is product number 1 and reactant number 2
```

[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

Model

typecode = SBML_MODEL

SBML Level 1

Version 1		Version 2	
Fieldname	**Type**	**Fieldname**	**Type**
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 1		Version 2	
Fieldname	**Type**	**Fieldname**	**Type**
typecode	as above	typecode	as above
metaid	string	metaid	string
notes	string	notes	string
annotation	string	annotation	string

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