## SimBiology<sup>®</sup> 2 Reference

# MATLAB®



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SimBiology<sup>®</sup> Reference

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# **Function Reference**

Modeling, Simulation, and Analysis Tools (p. 1-2)	Modeling, simulation, and analysis tools
Project Opening and Saving (p. 1-3)	Save and open projects in $MATLAB^{\ensuremath{\mathbb{R}}}$
SBML Model Reading and Writing (p. 1-4)	Export and Import SBML models
Object Construction (p. 1-5)	Create SimBiology <sup>®</sup> objects
Units and Unit Prefixes (p. 1-6)	Perform Unit conversion and create user-defined units

## Modeling, Simulation, and Analysis Tools

sbioconsmoiety	Find conserved moieties in SimBiology model
sbiodesktop	Open SimBiology modeling and simulation GUI
sbioensembleplot	Show results of ensemble run using 2-D or 3-D plots
sbioensemblerun	Multiple stochastic ensemble runs of SimBiology model
sbioensemblestats	Get statistics from ensemble run data
sbiogetmodel	Get model object that generated simulation data
sbiogetnamedstate	Get state and time data from simulation results
sbiohelp	Help for SimBiology functions
sbiolasterror	SimBiology last error message
sbiolastwarning	SimBiology last warning message
sbioparamestim	Perform parameter estimation
sbioplot	Plot simulation results in one figure
sbioreset	Delete all model and simulation objects
sbioselect	Search for objects with specified constraints
sbiosimulate	Simulate model object
sbiosubplot	Plot simulation results in subplots
sbioupdate	Update SimBiology model version

## **Project Opening and Saving**

sbioaddtolibrary	Add to user-defined library
sbiocopylibrary	Copy library to disk
sbioloadproject	Load project from file
sbioremovefromlibrary	Remove abstract kinetic law, unit, or unit prefix from library
sbiosaveproject	Save all models in root object
sbiowhos	Show contents of project file, library file, or SimBiology root object

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## **SBML Model Reading and Writing**

sbmlexport

sbmlimport

Export SimBiology model to SBML file

Import SBML-formatted file

## **Object Construction**

sbioabstractkineticlaw sbiomodel sbioroot sbiovariant Construct abstract kinetic law object Construct model object Return SimBiology root object Construct variant object 1

## **Units and Unit Prefixes**

sbioconvertunits

 ${\tt sbioregisterunitprefix}$ 

sbioshowunitprefixes

sbioshowunits

sbiounit

sbiounitcalculator

sbiounitprefix

Convert unit and unit value to new unit

Create user-defined unit prefix

Show unit prefixes in library

Show units in library

Create user-defined unit

Convert value between units

Create user-defined unit prefix

# Functions — Alphabetical List

Purpose	Construct abstract kinetic law object	
Syntax	<pre>abstkineticlawObj = sbioabstractkineticlaw('Name') abstkineticlawObj = sbioabstractkineticlaw('Name',     'Expression') abstkineticlawObj = sbioabstractkineticlaw('PropertyName', PropertyValue)</pre>	
Arguments	Name	Enter a name for the abstract kinetic law. Name must be unique in the user-defined kinetic law library. Name is referenced by <i>kineticlawObj</i> .
	Expression	The mathematical expression that defines the kinetic law.
Description	A SimBiology abstract kinetic law defines a reaction rate expression, species variables, and parameter variables for a kinetic law. <i>abstkineticlawObj</i> = sbioabstractkineticlaw(' <i>Name</i> ') creates an abstract kinetic law object, with the name <i>Name</i> and returns it to <i>abstkineticlawObj</i> .	
	The <i>abstract kinetic law</i> provides a mechanism for applying a specific rate law to multiple reactions. It acts as a mapping template for the reaction rate. The abstract kinetic law defines a reaction rate expression, which is shown in the property Expression, and the species and parameter variables used in the expression. The species variables are defined in the SpeciesVariables property, and the parameter variables are defined in the ParameterVariables property of the abstract kinetic law object.	
	In order to use <i>abstkineticlawObj</i> when constructing a kinetic law object with the method addkineticlaw, <i>abstkineticlawObj</i> must be added to the user-defined library with the sbioaddtolibrary function. To get the abstract kinetic law objects in the user-defined library, use the command get(sbioroot, 'UserDefinedKineticLaws').	

<pre>abstkineticlawObj = sbioabstractkineticlaw('Name','Expression') constructs a SimBiology abstract kinetic law object, abstkineticlawObj with the name 'Name' and with the expression 'Expression' and returns it to abstkineticlawObj.</pre>
<pre>abstkineticlawObj = sbioabstractkineticlaw('PropertyName', PropertyValue) defines optional properties. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).</pre>

Additional *abstkineticlawObj* properties can be viewed with the get command. *abstkineticlawObj* properties can be modified with the set command.

Method	delete (any object)	Delete SimBiology object
Summary	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	set (any object)	Set object properties
Property	Annotation	Store link to URL or file
Summary	Expression	Expression to determine reaction rate equation
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	ParameterVariables	Parameters in abstract kinetic law
	Parent	Indicate parent object
	SpeciesVariables	Species in abstract kinetic law

	Tag	Specify label for object	SimBiology
	Туре	Display top-leve object type	el SimBiology
	UserData	Specify data to a object	associate with
Examples	1 Create an abstract kinetic law.		
	abstkineticlawObj = sbioabstract	kineticlaw('ex_myla	w1', '(k1*s)/(k2+k1+s)');
	<b>2</b> Assign the parameter and specie	s variables in the	expression.
	set (abstkineticlawObj set (abstkineticlawObj		ubles', {'s'}); riables', {'k1', 'k2'});
	<b>3</b> Add the new abstract kinetic law	v to the user-defin	ied library.
	sbioaddtolibrary(abstk	ineticlawObj);	
	sbioaddtolibrary adds the abst library. You can verify this using		o the user-defined
	sbiowhos -kineticlaw -use	rdefined	
	SimBiology Abstract Kinet	ic Law Array	
	Index: Library: 1 UserDefined	Name: ex_mylaw1	Expression: (k1*s)/(k2+k1+s)
	<b>4</b> Use the new abstract kinetic law law.	when defining a	reaction's kinetic
		ction(modelObj,	'A + B <-> B + C'); ionObj, 'ex_mylaw1');

**Note** Remember to specify the SpeciesVariableNames and the ParameterVariableNames in kineticlawObj to fully define the ReactionRate of the reaction.

See Also addkineticlaw, addparameter, addreaction, sbiomodel

## sbioaddtolibrary

Purpose	Add to user-defined library		
Syntax	sbioaddtolibrary (abs sbioaddtolibrary (uni sbioaddtolibrary (uni	tObj)	
Arguments	abstkineticlawObj	Specify the abstract kinetic law object. The Name of the abstract kinetic law must be unique in the user-defined kinetic law library. Name is referenced by <i>kineticlawObj</i> . For more information about creating <i>kineticlawObj</i> , see sbioabstractkineticlaw.	
	unitObj	Specify the user-defined unit to add to the library. For more information about creating <i>unitObj</i> , see sbiounit.	
	unitprefixObj	Specify the user-defined unit prefix to add to the library. For more information about creating <i>unitprefixObj</i> , see sbiounitprefix.	
Description	The function sbioaddt unit prefixes to the use	olibrary adds abstract kinetic laws, units, and r-defined library.	
		<i>tkineticlawObj</i> ) adds the abstract kinetic law wObj) to the user-defined library.	
	sbioaddtolibrary ( <i>unitObj</i> ) adds the user-defined unit (unitObj) to the user-defined library.		
	<pre>sbioaddtolibrary (unitprefixObj) adds the user-defined unit prefix (unitprefixObj) to the user-defined library.</pre>		
		y function adds any abstract kinetic law, unit, ot object's UserDefinedLibrary property. These	

	library compon sessions.	ents become availa	able automat	ically in future MATLAB
		•		lt-in and user-defined e method addkineticlaw.
		(sbioroot, 'Bui		fined libraries, use the ') and (get(sbioroot,
	the function st	• 1	rary. You ca	er-defined library, use nnot remove an abstract object.
Examples	This example s to the user-def		e an abstract	kinetic law and add it
	1 Create an a	bstract kinetic law		
	abstkineti	.clawObj = sbioabstra	ctkineticlaw(	'ex_mylaw1', '(k1*s)/(k2+k1+s)');
	<b>2</b> Assign the p	parameter and spec	ies variables	in the expression.
				riables', {'s'}); Variables', {'k1', 'k2'});
	<b>3</b> Add the new	w abstract kinetic l	aw to the use	er-defined library.
	sbioaddt	olibrary(abstki	neticlawObj	);
		adds the abstract ify this using sbio		o the user-defined library.
	sbiowhos	s -kineticlaw -u	serdefined	
	SimBiolo	ogy Abstract Kin	etic Law Ar	ray
	Index: 1	Library: UserDefined	Name: mylaw1	Expression: (k1*s)/(k2+k1+s)

**4** Use the new abstract kinetic law when defining a reaction's kinetic law.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'A + B <-> B + C');
kineticlawObj = addkineticlaw(reactionObj, 'ex_mylaw1');
```

**Note** Remember to specify the SpeciesVariableNames and the ParameterVariableNames in kineticlawObj to fully define the ReactionRate of the reaction.

**See Also** addkineticlaw, sbioabstractkineticlaw, sbioremovefromlibrary, sbioroot, sbiounit, sbiounitprefix

Purpose	Find conserved moieties in SimBiology model		
Syntax	<pre>[G, Sp] = sbioconsmoiety(modelObj) [G, Sp] = sbioconsmoiety(modelObj, alg) H = sbioconsmoiety(modelObj, alg,'p') H = sbioconsmoiety(modelObj, alg,'p', FormatArg) [SI, SD, LO, NR, ND] = sbioconsmoiety(modelObj,'link')</pre>		
Arguments	G	An $m$ -by-n matrix, where $m$ is the number of conserved quantities found and $n$ is the number of species in the model. Each row of $G$ specifies a linear combination of species whose rate of change over time is zero.	
	Sp	Cell array of species names that labels the columns of G. If the species are in multiple compartments, species names are qualified with the compartment name in the form compartmentName.speciesName. For example, nucleus.DNA, cytoplasm.mRNA.	
	model0bj	Model object to be evaluated for conserved moieties.	
	alg	Specify algorithm to use during evaluation of conserved moieties. Valid values are 'qr', 'rreduce', or 'semipos'.	
	Н	Cell array of strings containing the conserved moieties.	
	р	Prints the output to a cell array of strings.	
	FormatArg	Specifies formatting for the output <i>H. FormatArg</i> should either be a C-style format string, or a positive integer specifying the maximum number of digits of precision used.	
	SI	Cell array containing the names of independent species in the model.	

	SD	Cell array containing the names of dependent species in the model.	
	LO	Link matrix relating SI and SD. The link matrix <i>LO</i> satisfies ND = LO*NR. For the 'link' functionality, species with their BoundaryCondition or ConstantAmount properties set to true are treated as having stoichiometry of zero in all reactions.	
	NR	Reduced stoichiometry matrices containing one row for each independent species. The concatenated matrix [NR;ND] is a row-permuted version of the full stoichiometry matrix of <i>mode10bj</i> .	
	ND	Reduced stoichiometry matrices containing one row for each dependent species. The concatenated matrix [ <i>NR</i> ; <i>ND</i> ] is a row-permuted version of the full stoichiometry matrix of <i>modelObj</i> .	
Description		consmolety(modelObj) calculates a complete set of linear ations for the species in the SimBiology model object	
	sbioconsmoiety computes conservation relations by analyzing the structure of the model object's stoichiometry matrix. Thus, sbioconsmoiety does not include species that are governed by algebraic or rate rules.		

[G, Sp] = sbioconsmoiety(modelObj, alg) provides an algorithm specification. For alg, specify 'qr', 'rreduce', or 'semipos'.

- When you specify 'qr', sbioconsmolety uses an algorithm based on QR factorization. From a numerical standpoint, this is the most efficient and reliable approach.
- When you specify 'rreduce', sbioconsmoiety uses an algorithm based on row reduction, which yields better numbers for smaller models. This is the default.

• When you specify 'semipos', sbioconsmolety returns conservation relations in which all the coefficients are greater than or equal to 0, permitting a more transparent interpretation in terms of physical quantities.

For larger models, the QR-based method is recommended. For smaller models, row reduction or the semipositive algorithm may be preferable. For row reduction and QR factorization, the number of conservation relations returned equals the row rank degeneracy of the model object's stoichiometry matrix. The semipositive algorithm may return a different number of relations. Mathematically speaking, this algorithm returns a generating set of vectors for the space of semipositive conservation relations.

H = sbioconsmoiety(modelObj, alg, 'p') returns a cell array of strings
H containing the conserved quantities in modelObj.

H = sbioconsmolety(modelObj, alg, 'p', FormatArg) specifies
formatting for the output H. FormatArg should either be a C-style
format string, or a positive integer specifying the maximum number
of digits of precision used.

[SI, SD, LO, NR, ND] = sbioconsmoiety(modelObj,'link') uses a QR-based algorithm to compute information relevant to the dimensional reduction, via conservation relations, of the reaction network in modelObj.

#### **Examples** Example 1

This example shows conserved moieties in a cycle.

**1** Create a model with a cycle. For convenience use arbitrary reaction rates, as this will not affect the result.

```
modelObj = sbiomodel('cycle');
modelObj.addreaction('a -> b','ReactionRate','1');
modelObj.addreaction('b -> c','ReactionRate','b');
modelObj.addreaction('c -> a','ReactionRate','2*c');
```

**2** Look for conserved moieties.

#### Example 2

Explore semipositive conservation relations in the oscillator model.

modelObj = sbmlimport('oscillator'); sbioconsmoiety(modelObj,'semipos','p') ans = 'pol + pol\_OpA + pol\_OpB + pol\_OpC' 'OpB + pol\_OpB + pA\_OpB1 + pA\_OpB\_pA + pA\_OpB2' 'OpA + pol\_OpA + pC\_OpA1 + pC\_OpA2 + pC\_OpA\_pC' 'OpC + pol\_OpC + pB\_OpC1 + pB\_OpC2 + pB\_OpC\_pB'

See Also "Moiety Conservation" in the SimBiology User's Guide documentation SimBiology method getstoichmatrix

Purpose	Convert unit and unit value to new unit				
Syntax	sbioconvertuni	ts(Obj, 'unit'	)		
Description	on SimBiology of the *Units prop property. For ex	bject, <i>Obj</i> to th perty to <i>unit</i> ar cample, sbioco	e unit, <i>un</i> nd updates nverunits	the current *Uni it. This function the correspondi on a speciesOb nitialAmountUn	configures ng value j updates the
	object that conta contain a unit p objects. For exa configured to 1 a call to sbioconv	ains a unit prop roperty are con mple, if <i>Obj</i> is and InitialAm ertunits with	perty. The npartment a species o puntUnits <i>unit</i> spec	s. <i>Obj</i> must be a SimBiology object, parameter, and object with Initi configured to mo ified as molecule lAmountUnits is	ects that l species .alAmount le, after the e, speciesObj
Examples	Convert the uni mole.	ts of the initial	amount o	f glucose from mo	lecule to
	molecule.	-		ign an initial am	ount of 23
	modelObj = compObj = a	and prompt, typ sbiomodel('cell' ddcompartment(mod = addspecies (cod	); delObj, 'C'		lAmountUnits', 'molecule')
	SimBiology	Species Array			
	Index: 1	Compartment: C	Name: glucose	InitialAmount: 23	InitialAmountUnits: molecule

 $\label{eq:converting} \textbf{2} \ \text{Convert the InitialAmountUnits of glucose from molecule to mole.}$ 

```
sbioconvertunits (speciesObj, 'mole')
```

**3** Verify the conversion of units and InitialAmount value.

Units are converted from molecule to mole.

get (speciesObj, 'InitialAmountUnits')

ans =

mole

The InitialAmount value is changed.

get (speciesObj, 'InitialAmount')

ans =

3.8192e-023

See Also sbioshowunits

Purpose	Copy library to disk		
Syntax	sbiocopylibrary ('kineticlaw', <i>'LibraryFileName'</i> ) sbiocopylibrary ('unit', <i>'LibraryFileName'</i> )		
Description	<pre>sbiocopylibrary copies all user-defined abstract kinetic laws to a file. sbiocopylibrary ('kineticlaw','LibraryFileName') copies all user-defined abstract kinetic laws to the file LibraryFileName.sbklib and places the copied file in the current directory.</pre>		
	<pre>sbiocopylibrary ('unit','LibraryFileName') copies all user-defined units and unit prefixes to the file LibraryFileName.sbulib.</pre>		
	To get the abstract kinetic law objects in the built-in and user-defined libraries, use the commands get(sbioroot, 'BuiltInKineticLaws') and get(sbioroot, 'UserDefinedKineticLaws'). To add an abstract kinetic law to the user-defined library, use the method sbioaddtolibrary.		
	To add a unit to the user-defined library, use the sbioregisterunit function. To add a unit prefix to the user-defined library, use the sbioregisterunitprefix function.		
Examples	Create an abstract kinetic law, add it to the user-defined library, and then copy the user-defined kinetic law library to a .sbklib file.		
	Create an abstract kinetic law.		
	<pre>abstkineticlawObj = sbioabstractkineticlaw('mylaw1', '(k1*s)/(k2+k1+s)');</pre>		
	<b>2</b> Add the new abstract kinetic law to the user-defined library.		
	<pre>sbioaddtolibrary(abstkineticlawObj);</pre>		
	sbioaddtolibrary adds the abstract kinetic law to the user-defined library. You can verify this using sbiowhos.		
	sbiowhos -kineticlaw -userdefined		

	SimBiolo	gy Abstract Kin	etic Law A	rray	
	Index: 1	Library: UserDefined	Name: mylaw1	Expression: (k1*s)/(k2+k1+s)	
	<b>3</b> Copy the user-defined kinetic law library.				
	sbiocopy	library ('kinet	iclaw','my	LibFile')	
	4 Verify with sbiowhos.				
	sbiowhos	-kineticlaw my	LibFile		
See Also		rary, sbioabstrac initprefix, sbior		aw, sbioregisterunit, Library	

Purpose	Open SimBiology modeling and simulation GUI		
Syntax	sbiodesktop sbiodesktop( <i>modelObj</i> )		
Arguments	modelObjModel object or an array of model objects. Enter the variable name for a top-level SimBiology model object. If you enter an array of model objects, the SimBiology desktop opens with 		
Description	<ul> <li>sbiodesktop opens the SimBiology GUI, which lets you do the following:</li> <li>Build a SimBiology model using reaction pathways and enter kinetic data for the reactions.</li> <li>Import or export SimBiology models to and from the MATLAB workspace or from a Systems Biology Markup Language (SBML) file.</li> <li>Modify an existing SimBiology model.</li> <li>Simulate a SimBiology model.</li> <li>View results from the simulation.</li> <li>Create and/or modify user-defined units and unit prefixes.</li> <li>Create and/or modify user-defined abstract kinetic law objects.</li> <li>sbiodesktop(mode10bj) opens the SimBiology GUI with a top-level</li> </ul>		
Examples	<pre>SimBiology model object (mode10bj). A top-level SimBiology model object has its property Parent set to the SimBiology root object. Create a SimBiology model in the MATLAB workspace, and then open the GUI with the model. model0bj = sbiomodel('cell'); sbiodesktop(model0bj)</pre>		

See Also sbioroot

Purpose	Show results of ensemble run using 2-D or 3-D plots		
Syntax	sbioensembleplot( <i>simdataObj</i> ) sbioensembleplot( <i>simdataObj</i> , Names) sbioensembleplot( <i>simdataObj</i> , Names, Time) FH = sbioensembleplot( <i>simdataObj</i> , Names) FH = sbioensembleplot( <i>simdataObj</i> , Names, Time)		
Arguments	simdataObj	An object that contains simulation data. You can generate a <i>simdataObj</i> object using the function sbioensemblerun. All elements of <i>simdataObj</i> must contain data for the same states in the same model.	
	Names	Either a string or a cell array of strings. Names may include qualified names such as 'CompartmentName.SpeciesName' or 'ReactionName.ParameterName' to resolve ambiguities. Specifying {} for Names plots data for all states contained in simdataObj.	
	Time	A numeric scalar value. If the specified <i>Time</i> is not an element of the time vectors in <i>simdataObj</i> , then the function resamples <i>simdataObj</i> as necessary using linear interpolation.	
	FH	Array of handles to figure windows.	
Description	distribution of all sbioensemblerun	( <i>simdataObj</i> ) shows a 3-D shaded plot of time-varying logged states in the SimData array <i>simdataObj</i> . The function plots an approximate distribution created by istribution to the data at every time step.	
	<pre>sbioensembleplot(simdataObj, Names) plots the distribution for the data specified by Names.</pre>		

	<pre>sbioensembleplot(simdataObj, Names, Time) plots a 2-D histogram of the actual data of the ensemble distribution of the states specified by Names at the particular time point Time.</pre>
	FH = sbioensembleplot( <i>simdataObj</i> , <i>Names</i> ) returns an array of handles $FH$ , to the figure window for the 3-D distribution plot.
	FH = sbioensembleplot( <i>simdataObj</i> , <i>Names</i> , <i>Time</i> ) returns an array of handles $FH$ , to the figure window for the 2-D histograms.
Examples	This example shows how to plot data from an ensemble run without interpolation.
	1 The project file, radiodecay.sbproj, contains a model stored in a variable called m1. Load m1 into the MATLAB workspace.
	<pre>sbioloadproject('radiodecay.sbproj','m1');</pre>
	2 Change the solver of the active configuration set to be ssa. Also, adjust the LogDecimation property on the SolverOptions property of the configuration set to reduce the size of the data generated.
	<pre>cs = getconfigset(m1, 'active'); set(cs, 'SolverType', 'ssa'); so = get(cs, 'SolverOptions'); set(so, 'LogDecimation', 10);</pre>
	<b>3</b> Perform an ensemble of 20 runs with no interpolation.
	<pre>simdataObj = sbioensemblerun(m1, 20);</pre>
	<b>4</b> Create a 2-D distribution plot of the species 'z' at time = 1.0.
	<pre>FH1 = sbioensembleplot(simdataObj, 'z', 1.0);</pre>
	<b>5</b> Create a 3-D shaded plot of both species.
	<pre>FH2 = sbioensembleplot(simdataObj, {'x','z'});</pre>
See Also	sbioensemblerun, sbioensemblestats, sbiomodel

## sbioensemblerun

#### Purpose Multiple stochastic ensemble runs of SimBiology model **Syntax** simdataObj = sbioensemblerun(modelObj, Numruns) simdataObj = sbioensemblerun(modelObj, Numruns, Interpolation) simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj) simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, Interpolation) simdataObj = sbioensemblerun(modelObj, Numruns, variantObj) simdataObj = sbioensemblerun(modelObj, Numruns, variantObj, Interpolation) simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj) simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj, Interpolation)

#### Arguments

simdataObj	An object that contains simulation data generated by sbioensemblerun. All elements of <i>simdataObj</i> must contain data for the same states in the same model.
mode10bj	Model object to be simulated.
Numruns	Integer scalar representing the number of stochastic runs to make.
Interpolation	String variable denoting the interpolation scheme to be used if data should be interpolated to get a consistent time vector. Valid values are 'linear' (linear interpolation), 'zoh' (zero-order hold), or 'off' (no interpolation). Default is 'off'. If interpolation is on, the data is interpolated to match the time vector with the smallest simulation stop time.

configsetObj	Specify the configuration set object to use in the ensemble simulation. For more information about configuration sets, see Configset object.
variant0bj	Specify the variant object to apply to the model during the ensemble simulation. For more information about variant objects, see Variant object.
simdataObj = sbioensemblerun( <i>modelObj</i> , <i>Numruns</i> ) performs a	

**Description** simdataObj = sbioensemblerun(modelObj, Numruns) performs a stochastic ensemble run of the SimBiology model object (modelObj), and returns the results in the SimData object (simdataObj). The active configset and the active variants are used during simulation and are saved in the output, SimData object (simdataObj).

sbioensemblerun uses the settings in the active configset on the model object (modelObj) to perform the repeated simulation runs. The SolverType property of the active configset must be set to one of the stochastic solvers: 'ssa', 'expltau', or 'impltau'. sbioensemblerun generates an error if the SolverType property is set to any of the deterministic (ODE) solvers.

simdataObj = sbioensemblerun(modelObj, Numruns, Interpolation)
performs a stochastic ensemble run of a model object (modelObj), and
interpolates the results of the ensemble run onto a common time vector
using the interpolation scheme (Interpolation).

simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj)
performs an ensemble run of a model object (modelObj), using the
specified configuration set (configsetObj).

simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, Interpolation) performs an ensemble run of a model object (modelObj), using the specified configuration set (configsetObj), and interpolates the results of the ensemble run onto a common time vector using the interpolation scheme (Interpolation). simdataObj = sbioensemblerun(modelObj, Numruns, variantObj)
performs an ensemble run of a model object (modelObj), using the
variant object or array of variant objects (variantObj).

simdataObj = sbioensemblerun(modelObj, Numruns, variantObj, Interpolation) performs an ensemble run of a model object (modelObj), using the variant object or array of variant objects (variantObj), and interpolates the results of the ensemble run onto a common time vector using the interpolation scheme (Interpolation).

simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj) performs an ensemble run of a model object (modelObj), using the configuration set (configsetObj), and the variant object or array of variant objects (variantObj). If the configuration set object (configsetObj) is empty, the active configset on the model is used for simulation. If the variant object (variantObj) is empty, then no variant (not even the active variants in the model) is used for the simulation.

simdataObj = sbioensemblerun(modelObj, Numruns, configsetObj, variantObj, Interpolation) performs an ensemble run of a model object (modelObj), using the configuration set (configsetObj), and the variant object or array of variant objects (variantObj), and interpolates the results of the ensemble run onto a common time vector using the interpolation scheme (Interpolation).

# **Examples** This example shows how to perform an ensemble run and generate a 2-D distribution plot.

1 The project file, radiodecay.sbproj, contains a model stored in a variable called m1. Load m1 into the MATLAB workspace.

sbioloadproject('radiodecay.sbproj','m1');

2 Change the solver of the active configset to be ssa. Also, adjust the LogDecimation property on the SolverOptions property of the configuration set.

```
cs = getconfigset(m1, 'active');
set(cs, 'SolverType', 'ssa');
```

```
so = get(cs, 'SolverOptions');
set(so, 'LogDecimation', 10);
```

**Tip** The LogDecimation property lets you define how often the simulation data is recorded as output. If your model has high concentrations or amounts of species, or a long simulation time (for example, 600s), you can record simulation data less often to manage the amount of data generated. Be aware that by doing so you might miss some transitions if your model is very dynamic. Try setting LogDecimation to 10 or more.

**3** Perform an ensemble of 20 runs with linear interpolation to get a consistent time vector.

```
simdata = sbioensemblerun(m1, 20, 'linear');
```

**4** Create a 2-D distribution plot of the species 'z' at a time = 1.0.

FH = sbioensembleplot(simdata, 'z', 1.0);

**See Also** addconfigset, getconfigset, sbioensemblestats, sbioensembleplot, setactiveconfigset, SimData object

Purpose	Get statistics from ensemble run data	
Syntax	<pre>[t,m] = sbioensemblestats(simDataObj) [t,m,v] = sbioensemblestats(simDataObj) [t,m,v,n] = sbioensemblestats(simDataObj)</pre>	
Arguments		
	t	Vector of doubles that holds the common time vector after interpolation.
	m	Matrix of mean values from the ensemble data. The number of rows in $m$ is the length of the common time vector $t$ after interpolation and the number of columns is equal to the number of species. The species order corresponding to the columns of $m$ can be obtained from any of the SimData objects in <i>simDataObj</i> using sbiogetnamedstate.
	simDataObj	A cell array of SimData objects, where each SimData object holds data for a separate simulation run. All elements of <i>simDataObj</i> must contain data for the same states in the same model. When the time vectors of the elements of <i>simDataObj</i> are not identical, <i>simDataObj</i> is first resampled onto a common time vector (see <i>interpolation</i> below).
	V	Matrix of variance obtained from the ensemble data. $v$ has the same dimensions as $m$ .
	n	Cell array of strings that holds names whose mean and variance are returned in $m$ and $v$ , respectively. The number of elements in $n$ is the same as the number of columns of $m$ and $v$ . The order of names in $n$ corresponds to the order of columns of $m$ and $v$ .

	names	Either a string or a cell array of strings. names may include qualified names such as 'CompartmentName.SpeciesName' or 'ReactionName.ParameterName' to resolve ambiguities. If you specify empty {} for names, sbioensemblestats returns statistics on all time courses contained in simDataObj.
	interpolation	String variable denoting the interpolation method to be used if data is to be interpolated to get a consistent time vector. See resample for a list of interpolation methods. Default is 'off'. If interpolation is on, the data is interpolated to match the time vector with the smallest simulation stop time.
Description	<pre>[t,m] = sbioensemblestats(simDataObj) computes the time-dependent ensemble mean m of the ensemble data simDataObj obtained by running sbioensemblerun.</pre>	
	[t,m,v] = sbioensemblestats(simDataObj) computes the time-dependent ensemble mean <i>m</i> and variance <i>v</i> for the ensemble run data simDataObj.	
	time-dependent er data <i>simDataObj</i> .	ensemblestats( $simDataObj$ ) computes the asemble mean $m$ and variance $v$ for the ensemble run Each column of $m$ or $v$ describes the ensemble mean as a function of time.
Examples		adiodecay.sbproj, contains a model stored in a Load m1 into the MATLAB workspace.
	1 Load a SimBio	logy model m1 from a SimBiology project file.
	sbioloadpro	oject('radiodecay.sbproj','m1');

2 Change the solver of the active configuration set to be ssa. Also, adjust the LogDecimation property on the SolverOptions property of the configuration set.

```
cs = getconfigset(m1, 'active');
set(cs, 'SolverType', 'ssa');
so = get(cs, 'SolverOptions');
set(so, 'LogDecimation', 10);
```

**3** Perform an ensemble of 20 runs with no interpolation.

simDataObj = sbioensemblerun(m1, 20);

**4** Get ensemble statistics for all species using the default interpolation method.

[T,M,V] = sbioensemblestats(simDataObj);

**5** Get ensemble statistics for a specific species using the default interpolation scheme.

[T2,M2,V2] = sbioensemblestats(simDataObj, {'z'});

**See Also** sbioensemblerun, sbioensembleplot, sbiogetnamedstate, sbiomodel

# sbioevent

Purpose	Construct event object	
	<b>Note</b> sbioevent has been removed and produces an error. Use addevent instead.	
Syntax		ggerValue, EventFcnsValue) 'PropertyName', PropertyValue)
Arguments	TriggerValue	Required property to specify a trigger condition. Must be a MATLAB expression that evaluates to a logical value.
	EventFcnsValue	A string or a cell array of strings, each of which specifies an assignment of the form 'objectname = expression', where objectname is the name of a valid SimBiology object.
	PropertyName	Property name for an event object from "Property Summary" on page 2-29.
	PropertyValue	Property value. For more information on property values, see the property reference for each property listed in "Property Summary" on page 2-29.
Description	SimBiology event object, a	aggerValue, EventFcnsValue) creates a assigns a value ( <i>TriggerValue</i> ) for the a value ( <i>EventFcnsValue</i> ) to the property ne object (eventObj).
	During model simulation, an event is triggered and its EventFcns are evaluated when the Trigger transitions from false to true. In order for an event to be used in a simulation, the event object must be added to a SimBiology model object with the copyobj function.	

	User's Guide documentation. event0bj = sbioevent('Proper optional properties. The property p	ent function. Idled during a simulation, see les Using Events" in the SimBiology tyName', PropertyValue) defines name/property value pairs can be any set (for example, name-value string
Method Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	set (any object)	Set object properties
Property Summary	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	EventFcns	Event expression
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Тад	Specify label for SimBiology object

### sbioevent

	Trigger	Event trigger		
	Туре	Display top-level SimBiology object type		
	UserData	Specify data to associate with object		
Examples	1 Create an event object.			
	eventObj = sbioeven	t('time>= 5', 'OpC = 200');		
	<b>2</b> Get a list of properties for	the event object.		
	get(eventObj)			
	MATLAB displays a list of event properties.			
	Active:	1		
	Annotation:	1.1		
		{ 'OpC = 200 ' }		
	Name:			
	Notes:	1.1		
	Parent:	[1x1 SimBiology.Model]		
	Tag:	1.1		
	Trigger:	'time >= 5'		
	Type:	'event'		
	UserData:	[]		
Soo Alco	addawant appyahi Fyant .			

See Also addevent, copyobj, Event object

Purpose	Get model object that generated simulation data	
Syntax	<i>modelObj</i> = sbiogetmo	del(simDataObj)
Arguments	simDataObj modelObj	SimData object returned by the function sbiosimulate or by sbioensemblerun. Model object associated with the SimData object.
Description	<pre>modelObj = sbiogetmodel(simDataObj) returns the SimBiology model (modelObj) associated with the results from a simulation run (simDataObj). You can use this function to find the model object associated with the specified SimData object when you load a project with several model objects and SimData objects.</pre>	
		del used to generate the SimData object urrently loaded, <i>mode10bj</i> is empty.
Example	Retrieve the model ob	ject that generated the SimData object.
	1 Create a model obj SimData object.	ect, simulate, and then return the results as a
	-	limport('oscillator'); biosimulate(modelObj);
	<b>2</b> Get the model that	generated the simulation results.
	-	piogetmodel(simDataObj) Wel - Oscillator
	Model Componer Models: Parameters: Reactions:	ots: 0 0 42

Rules: 0 Species: 23

**3** Check that the two models are the same.

modelObj == modelObj2
ans =
1

See Also sbiosimulate

Purpose	Get state and time data from simulation results		
	<b>Note</b> sbiogetnamedstate produces a warning and will be removed in a future version. Use selectbyname instead.		
Syntax	<pre>[t,x] = sbiogetnamedstate(simDataObj) [t,x] = sbiogetnamedstate(simDataObj,'Name') [t,x,Name] = sbiogetnamedstate()</pre>		
Description	<b>sbiogetnamedstate</b> returns state and time data from simulation results. $[t,x]$ = sbiogetnamedstate( <i>simDataObj</i> ) returns the time and state data associated with the simulation results ( <i>simDataObj</i> ) and returns to t and x respectively. <i>simDataObj</i> is a SimData object returned by the sbiosimulate function.		
	• $t$ is an n-by-1 vector of time samples labeling the rows of $x$ .		
	• x is an n-by-m matrix, where n is the number of times the reactions fired and m is the number of states logged during simulation. Each column of x defines the variation in the quantity of a species over time.		
	[t,x] = sbiogetnamedstate(simDataObj, 'Name') returns the state data associated with the name Name from the SimData object (smDataObj), and returns it to x. Name can be a cell array names. If a name, Name, does not exist, you see a warning.		
	[t,x,Name] = sbiogetnamedstate() returns the names associated with each column of x to Name.		
See Also	sbiosimulate		

# sbiogetsensmatrix

Purpose	3-D sensitivity r	natrix from simulation results
	-	ensmatrix produces a warning and will be removed in . Use getsensmatrix instead.
Syntax		ofacs] = sbiogetsensmatrix(simDataObj) opfacs] = sbiogetsensmatrix(imDataobj, opFacNames)
Arguments	Т	Column vector of length m specifying time points for the sensitivity data in <i>R</i> .
	R	An m-by-n-by-p array of sensitivity data with times, outputs, and input factors labeling its first, second, and third dimensions respectively.
	Outputs	Contains names of the species states that label the second dimension of <i>R</i> . R(:,i,j) is the time course for the sensitivity of state <i>Outputs</i> { <i>i</i> } to the input factor <i>Inpfacs</i> { <i>j</i> }. When <i>simdataObj</i> contains more than one element, the output arguments are cell arrays in which each cell contains data for the corresponding element of <i>simdataObj</i> .
	Inpfacs	Contains names of the input factors that label the third dimension of <i>R</i> . R(:,i,j) is the time course for the sensitivity of states <i>Outputs</i> { <i>i</i> } to the input factor <i>Inpfacs</i> { <i>j</i> }.
	simDataObj	SimData object returned by sbiosimulate. Contains sensitivity data when sensitivity analysis is enabled.

	OutNames	Specify outputs to get sensitivity data from <i>simDataObj</i> . Can be an empty array, or a single name, or a cell array of names. When an empty array is specified, returns the sensitivity data on all species states contained in <i>simDataObj</i> .
	InpFacNames	Specify input factors to get sensitivity data from <i>simDataObj</i> . Can be an empty array, or a single name, or a cell array of names. When an empty array is specified, returns the sensitivity data for all input factors contained in <i>simDataObj</i> .
Description	<pre>[T,R,States,Inpfacs] = sbiogetsensmatrix(simDataObj) gets time and sensitivity data from the SimData object simDataObj generated by simulating a SimBiology model object using sbiosimulate. sbiogetsensmatrix can only return sensitivity data that is contained in simDataObj.</pre>	
	time by the active Note that the sen	ta that is logged in <i>simDataObj</i> is set at simulation configuration set that is used during the simulation. sitivity data <i>R</i> returned by sbiogetsensmatrix may specified at simulation time.
	InpFacNames) gets	<pre>facs] = sbiogetsensmatrix(imDataobj, OutNames, sensitivity data for the outputs specified by OutNames cors specified by InpFacNames.</pre>
See Also	getsensmatrix,	sbiogetnamedstate, sbiohelp, sbiosimulate

# sbiohelp

Purpose	Help for SimBiology functions	
Syntax	<pre>sbiohelp('FunctionName') h = sbiohelp ('FunctionName')</pre>	
Description	<pre>sbiohelp('FunctionName') displays information for a SimBiology function (FunctionName).</pre>	
	h = sbiohelp (' <i>FunctionName</i> ') returns the help for the SimBiology function <i>FunctionName</i> to h.	
	You can get general information on the SimBiology software by specifying <i>FunctionName</i> as 'sbio'. General information about a SimBiology object can be returned by specifying <i>FunctionName</i> as or of the following:	
	• 'AbstractKineticLaw'	
	• 'KineticLaw'	
	• 'Model'	
	• 'Parameter'	
	• 'Reaction'	
	• 'Root'	
	• 'Rule'	
	• 'Species'	
	• 'Configset'	
	• 'CompileOptions'	
	<ul> <li>'ExplicitTauSolverOptions'</li> </ul>	
	<ul> <li>'ImplicitTauSolverOptions'</li> </ul>	
	• 'ODESolverOptions'	
	• 'RuntimeOptions'	
	• 'SSASolverOptions'	

Examples	<pre>sbiohelp('addreaction') sbiohelp addreaction</pre>
	sbiohelp reaction
	<pre>sbiohelp('sbioshowunits')</pre>

See Also MATLAB function help

# sbiolasterror

Purpose	SimBiology last error message	
Syntax	<pre>sbiolasterror diagstruct = sbiolasterror sbiolasterror([]) sbiolasterror(diagstruct)</pre>	
Arguments	diagstruct	The diagnostic structure holding Type, Message ID, and Message for the errors.
Description	<pre>sbiolasterror or diagstruct = sbiolasterror return a SimBiology diagnostic structure array containing the last error(s) generated by the software. The fields of the diagnostic structure are:</pre>	
	Туре	'error'
	MessageID	The message ID for the error (for example, 'SimBiology:ConfigSetNameClash')
	Message	The error message
		]) resets the SimBiology last error so that it will return antil the next SimBiology error is encountered.
		<i>iagstruct</i> ) will set the SimBiology last error(s) to those iagnostic structure ( <i>diagstruct</i> ).
Examples	This example she	ows how to use verify and sbiolasterror.
	I Import a mode	əl.
	a = sbml	Limport('radiodecay.xml')
SimBiology M		ogy Model - RadioactiveDecay
	Model ( Model	Components: Ls: 0

Parameters:	1
Reactions:	1
Rules:	0
Species:	2

2 Change the ReactionRate of a reaction to make the model invalid.

```
a.reactions(1).reactionrate = 'x*y'
SimBiology Model - RadioactiveDecay
Model Components:
    Models: 0
    Parameters: 1
    Reactions: 1
    Rules: 0
    Species: 2
```

**3** Use the function verify to validate the model.

```
a.verify
```

**4** Retrieve the error diagnostic struct.

```
p = sbiolasterror
p =
1x3 struct array with fields:
  Type
  MessageID
  Message
```

**5** Display the first error ID and Message.

```
p(1)
ans =
    Type: 'Error'
    MessageID: 'SimBiology:ReactionObjectDoesNotResolve'
    Message: 'The object 'y' in reaction 'Reaction1' does not
    resolve to any in-scope species or parameters.'
6 Reset the sbiolasterror.
    sbiolasterror([])
    ans =
      []
7 Set sbiolasterror to the diagnostic struct.
    sbiolasterror(p)
```

ans =

1x3 struct array with fields: Type MessageID Message

See Also sbiolastwarning, verify

# sbiolastwarning

Purpose	SimBiology last warning message		
Syntax	<pre>sbiolastwarning diagstruct = sbiolastwarning sbiolastwarning([]) sbiolastwarning(diagstruct)</pre>		
Arguments	diagstruct The diagnostic structure holding Type, Message ID, and Message for the warnings.		
Description	sbiolastwarning or <i>diagstruct</i> = sbiolastwarning return a SimBiology diagnostic structure array containing the last warnings generated by the software. The fields of the diagnostic structure are:		
	Type 'warning'		
	MessageID The message ID for the warning (for example, 'SimBiology:DANotPerformedReactionRate')		
	Message The warning message		
	<pre>sbiolastwarning([]) resets the SimBiology last warning so that it will return an empty array until the next SimBiology warning is encountered.</pre>		
	sbiolastwarning( <i>diagstruct</i> ) will set the SimBiology last warnings to those specified in the diagnostic structure ( <i>diagstruct</i> ).		
See Also	sbiolasterror, verify		

Purpose	Load project from file
Syntax	<pre>sbioloadproject('projFilename') sbioloadproject ('projFilename','variableName') sbioloadproject projFilename variableName1 variableName2 s = sbioloadproject ()</pre>
Description	<pre>sbioloadproject('projFilename') loads a SimBiology project from a project file (projFilename). If no extension is specified, sbioloadproject assumes a default extension of .sbproj. Alternatively, the command syntax is sbioloadproject projFilename.</pre>
	sbioloadproject (' <i>projFilename</i> ',' <i>variableName</i> ') loads only the variable variableName from the project file.
	sbioloadproject <i>projFilename variableName1 variableName2</i> loads the specified variables from the project.
	s = sbioloadproject () returns the contents of <i>projFilename</i> in a variable s. s is a struct containing fields matching the variables retrieved from the SimBiology project.
	You can display the contents of the project file using the sbiowhos command.
See Also	sbioaddtolibrary, sbioremovefromlibrary, sbiosaveproject, sbiowhos

Purpose	Construct model object		
Syntax	<pre>modelObj = sbiomodel('NameValue') modelObj = sbiomodel('PropertyName', PropertyValue)</pre>		
Arguments	NameValue		operty to specify a unique name for ect. Enter a character string.
	PropertyName		me for a Model object from ummary" on page 2-46.
	PropertyValue	Property va property.	lue. Valid value for the specified
Description	<pre>modelObj = sbiomodel('NameValue') creates a model object and returns the model object (modelObj). In the model object, this method assigns a value (NameValue) to the property Name.</pre>		
	<pre>modelObj = sbiomodel('PropertyName', PropertyValue) defines optional properties. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).</pre>		
	Simulate <i>modelObj</i> with the function sbiosimulate.		
	Add objects to a model object using the methods addkineticlaw, addmodel, addparameter, addreaction, addrule, and addspecies.		
	All SimBiology model objects can be retrieved from the SimBiology root object. A SimBiology model object has its Parent property set to the SimBiology root object.		
Method Summary	addcompartment (m compartment)		Create compartment object
	addconfigset (model)		Create configuration set object and add to model object

addevent (model)	Add event object to model object
addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
addreaction (model)	Create reaction object and add to model object
addrule (model)	Create rule object and add to model object
addvariant (model)	Add variant to model
copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
getadjacencymatrix (model)	Get adjacency matrix from model object
getconfigset (model)	Get configuration set object from model object
getstoichmatrix (model)	Get stoichiometry matrix from model object
getvariant (model)	Get variant from model
removeconfigset (model)	Remove configuration set from model
removevariant (model)	Remove variant from model
reorder (model, compartment)	Reorder component lists
set (any object)	Set object properties

	θ (	model object	
	verify (model, variant)	Validate and verify SimBiology model	
Property	Annotation	Store link to URL or file	
Summary	Compartments	Array of compartments in model or compartment	
	Events	Contain all event objects	
	Models	Contain all model objects	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	
	Parameters	Array of parameter objects	
	Parent	Indicate parent object	
	Reactions	Array of reaction objects	
	Rules	Array of rules in model object	
	Tag	Specify label for SimBiology object	
	Туре	Display top-level SimBiology object type	
	UserData	Specify data to associate with object	
Examples	1 Create a SimBiology model of		
	<pre>modelObj = sbiomodel(</pre>	'cell', 'Tag', 'mymodel');	
	<b>2</b> List all modelObj properties and the current values.		

setactiveconfigset (model)

Set active configuration set for

```
get(modelObj)
```

MATLAB returns:

```
Annotation: ''

Models: [Ox1 double]

Name: 'cell'

Notes: ''

Parameters: [Ox1 double]

Parent: [1x1 SimBiology.Root]

Species: [Ox1 double]

Reactions: [Ox1 double]

Rules: [Ox1 double]

Tag: 'mymodel'

Type: 'sbiomodel'

UserData: []
```

**3** Display a summary of modelObj contents.

model0bj

SimBiology Model - cell Model Components: Models: 0 Parameters: 0 Reactions: 0 Rules: 0 Species: 0

See Also addcompartment, addconfigset, addevent, addkineticlaw, addmodel, addparameter, addreaction, addrule, addspecies, copyobj, get, sbioroot, sbiosimulate, set

# sbioparamestim

Purpose	Perform parameter estimation		
Syntax	<pre>[k, result]= sbioparamestim(modelObj, tspan, xtarget, species_array, parameter_array) []= sbioparamestim(, species_array, parameter_array, k0) []= sbioparamestim(, species_array, parameter_array, k0, method)</pre>		
Arguments	k	Vector of estimated peremeter values	
		Vector of estimated parameter values.	
	result	struct with fields that provide information about the progress of optimization.	
	tspan	An n-by-1 vector representing the time span of the target data <i>xtarget</i> .	
	xtarget	An n-by-m matrix, where n is the number of time samples and m is the number of states you would like to match during the simulation. States can	

like to match during the simulation. States can
only be species varying with time. You cannot
use time varying (nonconstant) parameters. The
number of rows of <i>xtarget</i> must be the same as
the number of rows of <i>tspan</i> .

species array Either an array of species objects or a cell array of names of species in *modelObj* whose amounts should be matched during the estimation process. The length of the species array must be the same as the number of columns in *xtarget*. If there are species with duplicate names in different compartments, either use qualified names to identify the species correctly or use an array of species objects to identify the species correctly. sbioparamestim assumes that the order of the species in species array is the same as the order used to specify columns of *xtarget*. For example, a qualified name for a species named sp1 that is in a compartment named comp2 is comp2.sp1. parameter array Either an array of parameter objects or a cell array of names of parameters in modelObj whose values should be estimated. If you do not specify parameter array, sbioparamestim estimates all the parameters in the model. When a vector of parameter initial values (k0) is not specified, sbioparamestim takes the initial values from modelObj. When there are parameters with duplicate names, use either parameter objects or qualified parameter names to identify the right parameter object. For example, for a parameter named param1 used in a reaction named reaction1 and at the kinetic law level. the qualified name is reaction1.param1.

Array of doubles that holds initial values of parameters to be estimated. The length of <i>k0</i> is same as that of <i>parameter_array</i> . When you specify <i>k0</i> , sbioparamestim ignores any initial values specified in active variants attached to the model. If left unspecified, sbioparamestim takes initial values for parameters from the model ( <i>mode10bj</i> ) or, if there are active variants, sbioparamestim uses any initial values specified in the active variants. See Variant object for more information about variants.
Either a string or a cell array. If it is a string, it must be the name of the optimization algorithm to be used during the estimation process. Valid values are 'fminsearch', 'lsqcurvefit', 'lsqnonlin', 'fmincon', 'patternsearch', 'patternsearch_hybrid', 'ga', or 'ga_hybrid'.
If it is a cell array, it must have two elements: the first one is the name of the optimization method as described before and the second element is a MATLAB struct as returned by optimset, gaoptimset, or psoptimset.
sbioparamestim uses the cell array option to specify user-defined optimization options. If you do not specify this argument, then it defaults to 'lsqcurvefit' if the Optimization Toolbox™ is available; otherwise it defaults to 'fminsearch'.
'fminsearch' is a part of basic MATLAB and does not require the Optimization Toolbox. Note that 'fminsearch' is an unconstrained optimization method and this could result in negative values for parameters. In that case, use another optimization method.

#### **Description**[k, result]= sbioparamestim(modelObj, tspan, xtarget, species\_array, parameter\_array) estimates parameters of the SimBiology model object (modelObj), specified in parameter\_array, so as to match species given by species\_array with the target state (xtarget), whose time variation is given by the time span tspan. modelObj must be a top-level SimBiology model. A top-level SimBiology model object has its Parent property set to the SimBiology root object.

[...]= sbioparamestim(..., species\_array, parameter\_array, k0)
lets you specify the initial values of parameters.

[...]= sbioparamestim(..., species\_array, parameter\_array, k0, method) lets you specify the optimization method to use.

#### **Examples** Example 1

Given a model and some target data, estimate all of its parameters without having to specify any initial values. This is the simplest case. Estimate all of its parameters using the default method.

1 Load a model from the project, gprotein\_norules.sbproj. The project contains two models, one for the wild-type strain (stored in variable m1), and one for the mutant strain (stored in variable m2). Load the G protein model for the wild-type strain.

```
sbioloadproject gprotein_norules m1;
```

2 Store the target data in a variable.

```
Gt = 10000;
tspan = [0 10 30 60 110 210 300 450 600]';
Ga_frac = [0 0.35 0.4 0.36 0.39 0.33 0.24 0.17 0.2]';
xtarget = Ga_frac * Gt;
```

**3** Store all model parameters in an array.

p\_array = sbioselect(m1, 'Type', 'parameter');

**4** Store the species that should match target.

```
Ga = sbioselect(m1, 'Type', 'species', 'Name', 'Ga');
    % In this example only one species is selected.
    % To match more than one targeted species data
    % replace with selected species array.
5 Estimate the parameters.
     [k, result] = sbioparamestim(m1, tspan, xtarget, Ga, p array)
    k =
        0.1988
        0.0000
        0.0045
        6.2859
        0.0040
        0.9726
        0.0000
        0.1164
    result =
               fval: 8.7248e+005
           residual: [9x1 double]
           exitflag: 2
        iterations: 2
          funccount: 27
          algorithm: 'large-scale: trust-region reflective Newton'
            message: [1x77 char]
Example 2
```

Estimate parameters specified in p\_array and species specified in sp\_array using different algorithms. This example uses the data from "Example 1" on page 2-51.

```
[k1,r1] = sbioparamestim(m1, tspan, xtarget, Ga, p_array, ...
{}, 'fmincon');
[k2,r2] = sbioparamestim(m1, tspan, xtarget, Ga, p_array, ...
```

{}, 'patternsearch');
[k3,r3] = sbioparamestim(m1, tspan, xtarget, Ga, p\_array, ...
{}, 'ga')

#### Example 3

Estimate parameters specified in p\_array, species specified in sp\_array, and change default optimization options to use user-specified options. This example uses the data from "Example 1" on page 2-51.

```
myopt1 = optimset('Display','iter');
                     [k1,r1] = sbioparamestim(m1, tspan, xtarget, ...
                               sp array, p array, {},{'fmincon', myopt1});
                     myopt2.Tolmesh = 1.0e-4;
                     [k2,r2] = sbioparamestim(m1, tspan, xtarget, ...
                               sp array, p array, {},{'patternsearch', myopt2});
                     myopt3.PopulationSize = 50;
                     myopt3.Generations = 20;
                     [k3,r3] = sbioparamestim(m1, tspan, xtarget, ...
                               sp array, p array, {},{'ga', myopt3});
Reference
                  Tau-Mu Yi, Hiroaki Kitano, and Melvin I. Simon. PNAS (2003) vol.
                  100, 10764–10769.
See Also
                  SimBiology functions sbiomodel, sbiogetnamedstate
                  MATLAB function optimset
                  Genetic Algorithm and Direct Search Toolbox<sup>™</sup> functions gaoptimset,
                  psoptimset
```

# sbioparameter

Purpose	Construct parameter object		
	<b>Note</b> sbioparameter has been removed and produces an error. Use addparameter instead.		
Syntax	parameterObj = sbioparameter( <i>Obj</i> , <i>NameValue</i> ) parameterObj = sbioparameter(Obj, <i>NameValue</i> , <i>ValueValue</i> ) parameterObj = sbioparameter(' <i>PropertyName</i> ', <i>PropertyValue</i> )		
Arguments	Obj Model object or kinetic law object.		
	NameValue	Property for a parameter object. Enter a unique character string. Since objects can use this property to reference a parameter, a parameter object must have a unique name at the level it is created. For example, a kinetic law object cannot contain two parameter objects named kappa. However, the model object that contains the kinetic law object can contain a parameter object named kappa along with the kinetic law object.	
		You can use the function sbioselect to find an object with a specific Name property value.	
		For information on naming parameters, see Name.	
	ValueValue	Value of a parameter object. Enter a number.	
Description	<pre>parameterObj = sbioparameter(Obj, NameValue) constructs a SimBiology parameter object, enters a value (NameValue) for the required property Name, and returns the object (parameterObj).</pre>		
	To use a parameter object (paramaterObj) in a simulation, you must add the object to a SimBiology model, or kinetic law object with the method		

copyobj. You can use the addparameter method to simultaneously create and assign a parameter to a model or kinetic law object.

parameterObj = sbioparameter(Obj, NameValue, ValueValue) creates a parameter object, assigns a value (NameValue) to the property Name, assigns the value (ValueValue) to the property Value and returns the parameter object to a variable (parameterObj).

parameterObj = sbioparameter(...'PropertyName', PropertyValue...) defines optional properties. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).

Copy a SimBiology parameter object to a SimBiology model or kinetic law object with the method copyobj. Remove a parameter object from a model or kinetic law object with the method delete.

View additional parameter object properties with the get command. Modify additional parameter object properties with the set command. You can find help for parameterObj properties with the help *PropertyName* command and help for functions with the sbiohelp *FunctionName* command.

Method Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	rename (compartment, parameter, species)	Rename object and update expressions
	set (any object)	Set object properties

# sbioparameter

Property	Annotation	Store link to URL or file	
Summary	ConstantValue	Specify variable or constant parameter value	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	
	Parent	Indicate parent object	
	Тад	Specify label for SimBiology object	
	Туре	Display top-level SimBiology object type	
	UserData	Specify data to associate with object	
	Value	Assign value to parameter object	
	ValueUnits	Parameter value units	
Examples	Construct a parameter object. parameterObj = sbioparame % View the help for the p help(parameterObj, 'Value)	parameter object's Value property.	
	2 View parameter object properties.		
	get(parameterObj)		
	MATLAB returns:		
	Annotation: '' ConstantValue: 1 Name: 'kappa Notes: ''	a '	

Parent: [1x1 SimBiology.Reaction] Tag: '' Type: 'parameter' UserData: [] Value: 4 ValueUnits: '

**See Also** addparameter, copyobj, sbiomodel

# sbioplot

Purpose	Plot simulation results in one figure	
Syntax	sbioplot(simDataObj) sbioplot(simDataObj, fcnHandleValue, xArgsValue, yArgsValue)	
Arguments	simDataObj fcnHandleValue xArgsValue yArgsValue	SimBiology data object. Function handle. Cell array with the names of the states. Cell array with the names of the states.
Description	<pre>sbioplot(simDataObj) plots each simulation run for SimBiology data object, simDataObj, in the same figure. The plot is a time plot of each state in simDataObj. The figure also shows a hierarchical display of all the runs in a tree, with the ability of choosing which trajectories to show. sbioplot(simDataObj, fcnHandleValue, xArgsValue, yArgsValue) plots each simulation run for the SimBiology data object, simDataObj, in the same figure. The plot is created by calling the function handle, fcnHandleValue, with input arguments simDataObj, xArgsValue, and yArgsValue. xArgsValue and yArgsValue should be cell arrays with the names of the states. The function represented by the function handle should return an array of handles and names. The signature of the function is shown below. function [handles, names] = functionName(simDataObj, xArgsValue, YArgsValue)</pre>	
	The output argument handles is a two-dimensional array of handles to the lines plotted by the function. Each column corresponds to a run and each row corresponds to the lines being plotted for a state. names is a one-dimensional cell array that contains the names to be displayed on the nodes which are children of a Run Node. The length of names should be equal to the number of rows in the handles array returned.	

```
Examples This example shows how to plot data from an ensemble run without
interpolation.
% Load the radiodecay model.
    sbioloadproject('radiodecay.sbproj','m1');
    % Configure the model to run with the stochastic solver.
    cs = getconfigset(m1, 'active');
    set(cs, 'SolverType', 'ssa');
    set(cs.SolverOptions, 'LogDecimation', 100);
    % Run an ensemble simulation and view the results.
    simDataObj = sbioensemblerun(m1, 10, 'linear');
    sbioplot(simDataObj);
```

See Also sbiosubplot

# sbioreaction

Purpose	Construct reaction object		
	<b>Note</b> sbioreaction ha addreaction instead.	s been removed and produces an error. Use	
Syntax		tion('ReactantsValue',	
Arguments	ReactionValue	Specify the reaction equation. Enter a character string. A hyphen preceded by a space and followed by a right angle bracket (->) indicates reactants going forward to products. A hyphen with left and right angle brackets (<->) indicates a reversible reaction. Coefficients before reactant or product names must be followed by a space. Examples are 'A -> B', 'A + B -> C', '2 A + B -> 2 C', 'A <-> B'.	
	ReactantsValue	A string defining the species name, a cell array of strings, a species object or an array of species objects.	
	ProductsValue	A string defining the species name, a cell array of strings, a species object or an array of species objects.	

	RStoichCofficients	Stoichiometric coefficients for reactants, length of array equal to length of <i>ReactantsValue</i> .	
	PStoichCofficients	Stoichiometric coefficients for products, length of array equal to length of <i>ProductsValue</i> .	
<b>Description</b> reactionObj = sbioreaction('ReactionValue') creates a SimBio reaction object, assigns a value (ReactionValue) to the property Reaction, and returns the reaction object (reactionObj).		a value (ReactionValue) to the property	
	To use reactionObj in a simulation, you must add reactionObj to a SimBiology model object using copyobj. You can use addreaction to simultaneously create a reaction object and add it to a model object. A SimBiology model object is constructed with the function sbiomodel.		
	<pre>reactionObj = sbioreaction('ReactantsValue', 'ProductsValue') constructs a SimBiology reaction object that contains reactant species (Reactants) and product species (Products). The stoichiometric values are assumed to be 1. Reactants and Products can be a string defining the species name, a cell array of strings, a species object, or an array of species objects.</pre>		
	'ProductsValue', PStoid (RStoichCofficients) fo coefficients (PStoichCof Stoichiometry. The len	tion('ReactantsValue', RStoichCofficients, chCofficients) adds stoichiometric coefficients or reactant species, and stoichiometric ficients) for product species, to the property gth of Reactants and RCofficients must be Products and PCofficients must be equal.	
	defines optional properti can be in any format sup	tion('PropertyName', PropertyValue) es. The property name/property value pairs oported by the function set (for example, structures, and name-value cell array pairs).	
		nObj properties with the get command. Modify properties with the set command. You can find	

help for reactionObj properties with the help *PropertyName* command and help for functions with the sbiohelp *FunctionName* command.

A reaction object that does not have a parent can contain only species objects that do not have a parent. If a parented species object is added to an unparented reaction object, a copy of the species object will be made and added to the reaction as an unparented species.

When an unparented reaction object is added to a model, the method checks the model for the required species. If the model contains the species, the reaction object now uses the model's species object. If the model does not contain the species, the species object is added to the model and the reaction object uses it.

Method
Summary

у	addkineticlaw (reaction)	Create kinetic law object and add to reaction object
	addproduct (reaction)	Add product species object to reaction object
	addreactant (reaction)	Add species object as reactant to reaction object
	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	rmproduct (reaction)	Remove species object from reaction object products
	rmreactant (reaction)	Remove species object from reaction object reactants
	set (any object)	Set object properties

### sbioreaction

Property	
Summary	
-	

Active	Indicate object in use during simulation
Annotation	Store link to URL or file
KineticLaw	Show kinetic law used for ReactionRate
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Products	Array of reaction products
Reactants	Array of reaction reactants
Reaction	Reaction object reaction
ReactionRate	Reaction rate equation in reaction object
Reversible	Specify whether reaction is reversible or irreversible
Stoichiometry	Species coefficients in reaction
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

**Examples** 1 Construct reaction objects.

```
reactionObj1 = sbioreaction('a + 3 b -> 2 c');
reactionObj2 = sbioreaction({'a', 'b'}, [1 3], 'c', 2);
% View the help for the reaction object's Reversible property.
```

```
help(reactionObj1, 'Reversible')
2 View the property summary for reactionObj1.
  get(reactionObj1)
             Active: 1
         Annotation: ''
         KineticLaw: []
               Name: ''
              Notes: ''
         Parameters: [Ox1 double]
             Parent: []
           Products: [1x1 SimBiology.Species]
          Reactants: [2x1 SimBiology.Species]
           Reaction: 'a + 3 b -> 2 c'
       ReactionRate: ''
         Reversible: 0
      Stoichiometry: [-1 -3 2]
                Tag: ''
               Type: 'reaction'
           UserData: []
```

See Also

addreaction, sbiomodel

Purpose	Create user-defined unit			
	<b>Note</b> sbioregisterunit has been removed and produces an error. Use sbiounit followed by sbioaddtolibrary instead.			
Syntax	sbioregisterunit('Name', 'Composition', Multiplier) sbioregisterunit('Name', 'Composition', Multiplier, Offset)			
Description	<pre>sbioregisterunit('Name', 'Composition', Multiplier) creates a unit with the name Name, where the unit is defined as Multiplier*Composition and records the unit in the UserDefinedUnits vector of sbioroot and adds it to the user-defined library.</pre>			
	sbioregisterunit('Name', 'Composition', Multiplier, Offset) creates a unit with the specified offset. You can list available units with the sbioshowunits function.			
• <i>Name</i> is the name of the user-defined unit. <i>Name</i> must begin the characters and can contain characters, underscores or number can be any valid MATLAB variable name.				
	• Composition shows the combination of base and derived units that defines the unit Name. For example, molarity is mole/liter. Base units are the set of units used to define all unit quantity equations. Derived units are defined using base units or mixtures of base and derived units.			
	• <i>Multiplier</i> is the numerical value that defines the relationship between the unit <i>Name</i> and the base unit as a product of the <i>Multiplier</i> and the base unit. For example, 1 mole is 6.0221e23*molecule. The <i>Multiplier</i> is 6.0221e23.			
	<ul> <li>Offset is the numerical value by which the unit composition is modified from the base unit. For example, Celsius = (5/9)*( Fahrenheit-32); Multiplier is 5/9 and Offset is 32.</li> </ul>			

See Also sbioaddtolibrary, sbioremovefromlibrary, sbioshowunits, sbiounit

Purpose	Create user-defined unit prefix			
	<b>Note</b> sbioregisterunitprefix has been removed and produces an error. Use sbiounitprefix followed by sbioaddtolibrary instead.			
Syntax	<pre>sbioregisterunitprefix('NameValue', Exponent)</pre>			
Description	sbioregisterunitprefix(' <i>NameValue</i> ', <i>Exponent</i> ) creates a unit prefix with the name <i>NameValue</i> and with a multiplicative factor of 10^Exponent, and adds it to the UserDefinedUnitPrefixes vector in sbioroot and to the user-defined library. You can see the available unit prefixes with the sbioshowunitprefixes function.			
	• <i>NameValue</i> is the name of the prefix. Valid names must begin with a letter and can contain characters, underscores, or numbers. Built-in prefixes are defined based on the International System of Units (SI).			
	• <i>Exponent</i> shows the value of 10 <sup>Exponent</sup> that defines the relationship of the unit <i>Name</i> to the base unit. For example, for the unit picomole, Exponent is 12.			
See Also	sbioaddtolibrary, sbioremovefromlibrary, sbioshowunitprefixes, sbiounitprefix			

# sbioremovefromlibrary

Purpose	Remove abstract kinetic law, unit, or unit prefix from library			
Syntax	sbioremovefromlibrary (Obj) sbioremovefromlibrary ('Type', 'Name')			
Description	sbioremovefromlibrary (Obj) removes the abstract kinetic law, unit, or unit prefix object (Obj) from the user-defined library. The removed component will no longer be available automatically in future MATLAB sessions.			
	sbioremovefromlibrary does not remove an abstract kinetic law that is being used in a model.			
	You can use a built-in or user-defined abstract kinetic law when you construct a kinetic law object with the method addkineticlaw.			
	sbioremovefromlibrary ('Type', 'Name') removes the object of type 'Type' with name 'Name' from the corresponding user-defined library. Type can be 'kineticlaw', 'unit' or 'unitprefix'.			
	To get a component of the built-in and user-defined libraries, use the commands get(sbioroot, 'BuiltInLibrary') and get(sbioroot, 'UserDefinedLibrary').			
	To create an abstract kinetic law, unit, or unit prefix, use sbioabstractkineticlaw, sbiounit, or sbiounitprefix respectively.			
	To add an abstract kinetic law, unit, or unit prefix to the user-defined library, use the function sbioaddtolibrary.			
Example	This example shows how to remove an abstract kinetic law from the user-defined library.			
	1 Create an abstract kinetic law.			
	<pre>abstkineticlawObj = sbioabstractkineticlaw('mylaw1', '(k1*s)/(k2+k1+s)');</pre>			
	<b>2</b> Add the new abstract kinetic law to the user-defined library.			
	<pre>sbioaddtolibrary(abstkineticlawObj);</pre>			

sbioaddtolibrary adds the abstract kinetic law to the user-defined library. You can verify this using sbiowhos.

sbiowhos -kineticlaw -userdefined SimBiology Abstract Kinetic Law Array Index: Library: Name: Expression: 1 UserDefined mylaw1 (k1\*s)/(k2+k1+s)

**3** Remove the abstract kinetic law.

sbioremovefromlibrary('kineticlaw', 'mylaw1');

See Also sbioaddtolibrary, sbioabstractkineticlaw, sbiounit, sbiounitprefix

### sbioreset

Purpose	Delete all model and simulation objects			
Syntax	sbioreset			
Description	sbioreset deletes all SimBiology model and simulation objects at the root level. You cannot use a SimBiology model or simulation object after it is deleted. You should remove objects from the MATLAB workspace with the function clear.			
	The SimBiology root object contains a list of SimBiology model objects, available units, unit prefixes, and kinetic law objects. A SimBiology model object has its Parent property set to the SimBiology root object.			
	To add an abstract kinetic law to the SimBiology root user-defined library, use the sbioaddtolibrary function. To add a unit to the SimBiology user-defined library on the root, use the sbioregisterunit function. To add a unit prefix to the SimBiology user-defined library on the root, use the sbioregisterunitprefix function.			
Example	This example shows the difference between sbioreset and clear all.			
	I Import a model into the workspace.			
	<pre>modelObj = sbmlimport('oscillator');</pre>			
	Note that the workspace contains modelObj and if you query the SimBiology root, there is one model on the root object.			
	rootObj = sbioroot			
	SimBiology Root Contains:			
	Models: Builtin Abstract Kinetic Laws: User Abstract Kinetic Laws: Builtin Units: User Units: Builtin Unit Prefixes:	1 3 0 54 0 13		
	DUIILIN UNIL PRETIXES:	10		

User	Unit	Prefixes:	0	

**2** Use clear all to clear the workspace. The modelObj still exists on the rootObj.

clear all

root0bj

SimBiology Root Contains:

Models:	1
Builtin Abstract Kinetic Laws:	3
User Abstract Kinetic Laws:	0
Builtin Units:	54
User Units:	0
Builtin Unit Prefixes:	13
User Unit Prefixes:	0

**3** Usesbioreset to delete the modelObj from the root.

sbioreset rootObj

SimBiology Root Contains:

Models:	0
Builtin Abstract Kinetic Laws:	3
User Abstract Kinetic Laws:	0
Builtin Units:	54
User Units:	0
Builtin Unit Prefixes:	13
User Unit Prefixes:	0

See Also sbioroot

### sbioroot

Purpose	Return SimBiology root object	
Syntax	<i>rootObj</i> = sbioroot	
Arguments	rootObj Return sbi	coroot to this object.
Description	<i>rootObj</i> = sbioroot returns the SimBiology root object to root. The SimBiology root object contains a list of the top-level SimBiology model objects, available units, unit prefixes, and available abstract kinetic law objects.	
	The units define the set of built-in Unit object for more information	n units and user-defined units. See n.
	The unit prefixes define the set of built-in prefixes and user-defined prefixes. See Unit Prefix object for more information.	
	The abstract kinetic law objects define the built-in abstract kinetic law objects and user-defined abstract kinetic law objects. The process of defining a reaction requires the use of abstract kinetic law objects when configuring a SimBiology reaction object's KineticLaw property with the addkineticlaw function.	
	To add a unit, prefix or abstract kinetic law to the root (in the user-defined library), use the sbioaddtolibrary function. To remove, use sbioremovefromlibrary.	
	The models opened in the SimBiology desktop are stored in the root object.	
Method Summary	copyobj (any object)	Copy SimBiology object and its children
	get (any object)	Get object properties

### sbioroot

	reset (root)	Delete all model objects from root object
	set (any object)	Set object properties
Property Summary	BuiltInLibrary Models	Library of built-in components
	Туре	Contain all model objects Display top-level SimBiology object type
	UserDefinedLibrary	Library of user-defined components
See Also	addkineticlaw, sbiomodel, sbioreset	

### sbiorule

Purpose	Construct rule object		
	<b>Note</b> sbiorule l instead.	nas been removed and produces an error. Use addrule	
Syntax	-	lle('RuleValue') lle(RuleValue, 'RuleTypeValue') lle('PropertyName', PropertyValue)	
Arguments	RuleValue	Enter a character string within quotation marks. For example, enter the algebraic rule 'Va*Ea + Vi*Ei - K2'.	
	RuleTypeValue	Enter 'algebraic', 'initialassignment', 'repeatedAssignment', or 'rate'. See RuleType for more information.	
Description	A SimBiology rule is a mathematical expression that modifies a species amount, or a parameter value. A rule is a MATLAB expression that uses species, and parameters.		
	<i>ruleObj</i> = sbiorule(' <i>RuleValue</i> ') creates a rule object, assigns a value ( <i>RuleValue</i> ) to the property Rule, assigns the value 'algebraic' to the property RuleType, and assigns the root object to the property Parent.		
	object with the fu to a SimBiology r	n a simulation, ruleObj must be added to a model nction copyobj. Note that a rule can also be added nodel with the addrule function. A model object is the function sbiomodel.	
	-	le( <i>RuleValue</i> , ' <i>RuleTypeValue</i> ') in addition to the x enables you to specify RuleType.	
		es. The property name/property value pairs can be in	

any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).

View additional rule properties with the function get, and modify rule properties with the function set. View the rules in a model (modelObj) with get(modelObj, 'Rules').

Method Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	set (any object)	Set object properties
Property Summary	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Rule	Specify species and parameter interactions
	RuleType	Specify type of rule for rule object
	Тад	Specify label for SimBiology object

### sbiorule

Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

### **Examples** Example 1

Construct a rule object and copy it to a model object.

```
ruleObj = sbiorule('Enzt - Enzi - Enza)');
modelObj = sbiomodel('cell')
ruleObj_copy = copyobj(ruleObj, modelObj);
```

#### Example 2

View the help for the rule object's RuleType property.

help(ruleObj, 'RuleType')

#### **Example 3**

List the properties for a rule.

```
get(ruleObj)
```

```
Active: 1
Annotation: ''
Name: ''
Notes: ''
Parent: []
Rule: 'myrule'
RuleType: 'algebraic'
Tag: ''
Type: 'rule'
UserData: []
```

See Also

addrule, copyobj, sbiomodel

Purpose	Save all models in root object
Syntax	sbiosaveproject projFilename sbiosaveproject projFilename variableName sbiosaveproject projFilename variableName1 variableName2
Description	sbiosaveproject <i>projFilename</i> saves all models in the SimBiology root object to the binary SimBiology project file named <i>projFilename</i> .sbproj. The project can be loaded with sbioloadproject. sbiosaveproject returns an error if <i>projFilename</i> .sbproj is not writable.
	sbiosaveproject creates the binary SimBiology project file named simbiology.sbproj. sbiosaveproject returns an error if this is not writable.
	sbiosaveproject <i>projFilename variableName</i> saves only variableName. variableName can be a SimBiology model or any MATLAB variable.
	sbiosaveproject <i>projFilename variableName1 variableName2</i> saves the specified variables in the project.
	Use the functional form of sbiosaveproject when the file name or variable names are stored in a string. For example, if the file name is stored in the variable <i>fileName</i> and you want to store MATLAB variables <i>variableName1</i> and <i>variableName2</i> , type sbiosaveproject ( <i>projFileName</i> , ' <i>variableName1</i> ', ' <i>variableName2</i> ') at the command line.
Examples	1 Import an SBML file and simulate (default configset object is used).
	<pre>modelObj = sbmlimport ('oscillator.xml'); timeseriesObj = sbiosimulate(modelObj);</pre>
	<b>2</b> Save the model and the simulation results to a project.
	sbiosaveproject myprojectfile modelObj timeseriesObj

See Also sbioaddtolibrary, sbioloadproject, sbioremovefromlibrary, sbiowhos

Purpose	Search for objects wit	th specified constraints
Syntax	Out = sbioselect('W PropertyValue) Out = sbioselect(Ob Out = sbioselect(Ob PropertyValue)	ropertyName', PropertyValue) here', 'PropertyName', 'Condition', j, 'PropertyName', PropertyValue) j, 'Type', 'TypeValue', 'PropertyName',
	<pre>Out = sbioselect(Obj, 'Where', 'PropertyName', 'Condition', PropertyValue) Out = sbioselect(Obj, 'Where', 'PropertyName1', 'Condition1', PropertyValue1, 'Where', 'PropertyName2', 'Condition2', PropertyValue2,) Out = sbioselect(Obj, 'Depth', DepthValue,)</pre>	
Arguments	Out	Object or array of objects returned by the <b>sbioselect</b> function. <i>Out</i> might contain a mixture of object types (for example, species and parameters), depending on the selection you specify. If <i>PropertyValue</i> is a cell array, then the function returns all objects with the property ' <i>PropertyName</i> ' that matches any element of <i>PropertyValue</i> .
	Obj	SimBiology object or array of objects to search. If an object is not specified, sbioselect searches the root.
	PropertyName	Any property of the object being searched.
	PropertyValue	Specify <i>PropertyValue</i> to include in the selection criteria.
	TypeValue	Type of object to include in the selection, for example, sbiomodel, species, reaction, or kineticlaw.

	Condition	Constraint to impose on the search. See the table under "Description" on page 2-80 for a list of conditions.
	DepthValue	Specify the depth number to search. Valid numbers are positive integer values and inf. If <i>DepthValue</i> is inf, sbioselect searches <i>Obj</i> and all of its children. If <i>DepthValue</i> is 1, sbioselect only searches <i>Obj</i> and not its children. By default, <i>DepthValue</i> is inf.
Description	sbioselect searches	for objects with specified constraints.
	root object (including and returns the objec	ropertyName', PropertyValue) searches the all model objects contained by the root object) ts with the property name (PropertyName) and ertyValue) contained by the root object.
	PropertyValue) search	nere', 'PropertyName', 'Condition', les the root object and finds objects that have opertyName) and value (PropertyValue) that n (Condition).
		<i>i</i> , ' <i>PropertyName</i> ', <i>PropertyValue</i> ) returns the erty name ( <i>PropertyName</i> ) and property value nd in any object ( <i>Obj</i> ).
	PropertyValue) finds name (PropertyName) object (Obj). TypeVal	<i>i</i> , 'Type', ' <i>TypeValue</i> ', ' <i>PropertyName</i> ', the objects of type (TypeValue), with the property ) and property value ( <i>PropertyValue</i> ) found in any <i>ue</i> is the type of SimBiology object to be included xample, species, reaction, or kineticlaw.
	PropertyValue) finds o	i, 'Where', ' <i>PropertyName</i> ', 'Condition', bjects that have a property name ( <i>PropertyName</i> ) /alue) that match the condition (Condition).
	you must use the san	ing property value without specifying a condition, ne format as get returns. For example, if get MyObject', sbioselect will not find an object

with a Name property value of 'myobject'. Therefore, for this example, you must specify:

```
modelObj = sbioselect ('Name', 'MyObject')
```

Instead, if you use a condition, you can specify:

```
modelObj = sbioselect ('Where', 'Name', '==i', 'myobject')
```

Thus, conditions let you control the specificity of your selection.

sbioselect searches for model objects on the root in both cases.

The conditions, with examples of property names and corresponding examples of property values that you can use, are listed in the following tables. This table shows you conditions for numeric properties.

Conditions for Numeric Properties	Example Syntax
==	Search in the model object (modelObj), and return parameter objects that have Value equal to 0.5. sbioselect returns parameter objects because only parameter objects have a property called Value.
	parameterObj = sbioselect (modelObj, 'Where', 'Value', '==', 0.5)
	In the case of ==, this is equivalent to omitting the condition as shown:
	parameterObj = sbioselect (modelObj, 'Value', 0.5)
	Search in the model object (modelObj), and return parameter objects that have ConstantValue false (nonconstant parameters).
	parameterObj = sbioselect (modelObj, 'Where', 'ConstantValue', '==', false)
~=	Search in the model object (modelObj), and return parameter objects that do not have Value equal to 0.5.
	parameterObj = sbioselect (modelObj, 'Where', 'Value', '~=', 0.5)

Conditions for Numeric Properties	Example Syntax
>,<,>=,<=	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) greater than 50.
	<pre>speciesObj = sbioselect (modelObj, 'Where', 'InitialAmount', '&gt;', 50)</pre>
	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) less than or equal to 50.
	<pre>speciesObj = sbioselect (modelObj, 'Where', 'InitialAmount', '&lt;=', 50)</pre>
between	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) between 200 and 300.
	speciesObj = sbioselect (modelObj, 'Where', 'InitialAmount', 'between', [200 300])
~between	Search in the model object (modelObj), and return species objects that have an initial amount (InitialAmount) that is not between 200 and 300.
	<pre>speciesObj = sbioselect (modelObj, 'Where', 'InitialAmount', '~between', [200 300])</pre>

Conditions for String Properties	Example Syntax
==	Search in the model object (modelObj), and return species objects named 'Glucose'.
	speciesObj = sbioselect (modelObj, 'Type', 'species', 'Where', 'Name', '==', 'Glucose')
~=	Search in the model object (modelObj), and return species objects that are not named 'Glucose'.
	speciesObj = sbioselect (modelObj, 'Type', 'species', 'Where', 'Name', '~=', 'Glucose')
==i	Same as ==; in addition, this is case insensitive.
~=i	Search in the model object (modelObj), and return species objects that are not named 'Glucose', ignoring case.
	speciesObj = sbioselect (modelObj, 'Type', 'species', 'Where', 'Name', '~=i', 'glucose')

The following table shows you conditions for properties whose values are strings.

Conditions for String Properties	Example Syntax
regexp. Supports expressions supported by the functions regexp and regexpi.	<pre>Search in the model object (modelObj), and return objects that have 'ese' or 'ase' anywhere within the name. Obj = sbioselect (modelObj, 'Where', 'Name', 'regexp', '[ea]se') Search in the root, and return objects that have kinase anywhere within the name. Obj = sbioselect ('Where', 'Name', 'regexp', 'kinase') Note that this query could result in a mixture of object types (for example, species and parameters).</pre>
regexpi	Same as regexp; in addition, this is case insensitive.
~regexp	<pre>Search in the model object (modelObj), and return objects that do not have kinase anywhere within the name. Obj = sbioselect (modelObj, 'Where', 'Name', '~regexp', 'kinase')</pre>
~regexpi	Same as ~regexp; in addition, this is case insensitive.

The condition 'contains' can be used only for those properties whose values are an array of SimBiology objects. The following table shows you an example of using contains.

Condition	Example Syntax
'contains'	<pre>Search in the model object and return reaction objects whose Reactant property contains the specified species. Out = sbioselect(modelObj, 'Where', 'Reactants', 'contains', modelObj.Species(1))</pre>

Out = sbioselect(Obj, 'Where', 'PropertyName1', 'Condition1', PropertyValue1, 'Where', 'PropertyName2', 'Condition2', PropertyValue2,...) finds objects contained by Obj that matches all the conditions specified.

You can combine any number of property name/property value pairs and conditions in the sbioselect command.

Out = sbioselect(Obj, 'Depth', DepthValue,...) finds objects using a
model search depth of DepthValue.

### **Examples** 1 Import a model.

modelObj = sbmlimport('oscillator');

2 Find and return an object named pA.

Obj = sbioselect(modelObj, 'Name', 'pA');

**3** Find and return species objects whose Name starts with p and have A or B as the next letter in the name.

```
speciesObj = sbioselect(modelObj, 'Type', 'species', 'Where',...
'Name', 'regexp', '^p[AB]');
```

**4** Find a cell array. Note how cell array values must be specified inside another cell array.

```
See Also regexp
```

# sbioshowunitprefixes

Purpose	Show unit prefixes in library		
Syntax	<pre>UnitPrefixObjs = sbioshowunitprefixes [Name, Multiplier] = sbioshowunitprefixes [Name, Multiplier, Builtin] = sbioshowunitprefixes [Name, Multiplier, Builtin] = sbioshowunitprefixes('Name')</pre>		
Arguments	unitPrefixObjs	Vector of unit prefix objects from the BuiltInLibrary and UserDefinedLibrary properties of the Root object.	
	Name	Name of the built-in or user-defined unit prefix. Built-in prefixes are defined based on the International System of Units (SI).	
	Multiplier	Shows the value of 10 <sup>Exponent</sup> that defines the relationship of the unit prefix <i>Name</i> to the base unit. For example, the multiplier in picomole is 10e-12.	
	Builtin	An array of logical values. If <i>Builtin</i> is true for a unit prefix, the unit prefix is built in. If <i>Builtin</i> is false for a unit prefix, the unit prefix is user defined.	
Description	sbioshowunitprefixes returns information about unit prefixes in the SimBiology library.		
	<i>UnitPrefixObjs</i> = sbioshowunitprefixes returns the unit prefixes in the library as a vector of unit prefix objects in <i>UnitPrefixObjs</i> .		
	[ <i>Name, Multiplier</i> ] = sbioshowunitprefixes returns the multiplier for each prefix in <i>Name</i> to <i>Multiplier</i> as a cell array of strings.		
	[Name, Multiplier, Builtin] = sbioshowunitprefixes returns whether the unit prefix is built in or user defined for each unit prefix in Name to Builtin.		

	[ <i>Name, Multiplier, Builtin</i> ] = sbioshowunitprefixes(' <i>Name</i> ') returns the name, multiplier, and built-in status for the unit prefix with name <i>Name</i> can be a cell array of strings.	
Examples	[name, multiplier] = sbioshowunitprefixes; [name, multiplier] = sbioshowunitprefixes('nano');	
See Also	sbioconvertunits, sbioshowunits, sbiounitprefix	

### sbioshowunits

Show units in library		
<pre>unitObjs = sbioshowunits [Name, Composition] = sbioshowunits [Name, Composition, Multiplier] = sbioshowunits [Name, Composition, Multiplier, Offset] = sbioshowunits [Name, Composition, Multiplier, Offset, Builtin] = sbioshowunits [Name, Composition, Multiplier, Offset, Builtin] = sbioshowunits('Name')</pre>		

### Arguments

unitObjs	Vector of unit objects from the BuiltInLibrary and UserDefinedLibrary properties of the Root object.
Name	Name of the built-in or user-defined unit.
Composition	Shows the combination of base and derived units that defines the unit <i>Name</i> . For example, molarity is mole/liter.
Multiplier	The numerical value that defines the relationship between the unit <i>Name</i> and the base or derived unit as a product of the <i>Multiplier</i> and the base unit or derived unit. For example, 1 mole is 6.0221e23*molecule. The <i>Multiplier</i> is 6.0221e23.
Offset	Numerical value by which the unit composition is modified from the base unit. For example, Celsius = (5/9)*( Fahrenheit-32); <i>Multiplier</i> is 5/9 and Offset is 32.
Builtin	An array of logical values. If <i>Builtin</i> is true for a unit, the unit is built in. If <i>Builtin</i> is false for a unit, the unit is user defined.

Description	<i>unitObjs</i> = sbioshowunits returns the units in the library to <i>unitObjs</i> as a vector of unit objects.		
	[ <i>Name, Composition</i> ] = sbioshowunits returns the composition for each unit in <i>Name</i> to <i>Composition</i> as a cell array of strings.		
	[ <i>Name, Composition, Multiplier</i> ] = sbioshowunits returns the multiplier for the unit with name <i>Name</i> to <i>Multiplier</i> .		
	<pre>[Name, Composition, Multiplier, Offset] = sbioshowunits returns the offset for the unit with name Name to Offset. The unit is defined as Multiplier*Composition+Offset. [Name, Composition, Multiplier, Offset, Builtin] = sbioshowunits returns whether the unit is built in or user defined for each unit in Name to Builtin.</pre>		
	[Name, Composition, Multiplier, Offset, Builtin] = sbioshowunits('Name') returns the name, composition, multiplier, offset and built-in status for the unit with name Name. Name can be a cell array of strings.		
Examples	<pre>[name, composition] = sbioshowunits; [name, composition] = sbioshowunits('molecule');</pre>		
See Also	sbioconvertunits, sbioshowunitprefixes, sbiounit		

# sbiosimulate

Purpose	Simulate model object		
Syntax	<pre>[t,x,names] = sbiosimulate(modelObj) simDataObj = sbiosimulate(modelObj)  = sbiosimulate(modelObj, configsetObj)  = sbiosimulate(modelObj, variantObj)  = sbiosimulate(modelObj, configsetObj, variantObj)</pre>		
Arguments	Output Arguments		
	t	An n-by-1 vector of time points. Shows the simulation time steps.	
	X	An $n-by-m$ data array, where $n$ is the number of time samples and $m$ is the number of states logged in the simulation. Each column of x describes the variation in the quantity of a state over time.	
	names	An m-by-1 cell array of names. If the species are in multiple compartments, species names are qualified with the compartment name in the form compartmentName.speciesName. For example, nucleus.DNA, cytoplasm.mRNA.	
		Parameter names are qualified with the reaction name if the parameter is scoped to the reaction's kinetic law. For example, Transcription.k1, denotes that the parameter k1 is scoped to the kinetic law for the reaction Transcription.	
	simdataObj	An object that holds time and state data as well as metadata, such as the types and names for the logged states or the configuration set used during simulation. You can access time, data, and names stored in <i>simdataObj</i> through <i>simdataObj</i> properties. See SimData object for more information.	

### **Input Arguments**

	model0bj	Model object to be simulated.	
	configset0bj	Specify the configuration set object to use in the simulation. For more information about configuration sets, see Configset object.	
	variantObj	Specify the variant object to apply to the model during the simulation. For more information about variant objects, see Variant object.	
Description	<pre>[t,x,names] = sbiosimulate(modelObj) simulates a model object (modelObj) using the active configuration set attached to the model (modelObj) and returns the specified outputs as described in "Output Arguments" on page 2-92.</pre>		
	<pre>simDataObj = sbiosimulate(modelObj) simulates the Simbiology model object (modelObj) and returns the results to a SimData object.</pre>		
	<pre> = sbiosimulate(modelObj, configsetObj) simulates a model object (modelObj) using a configuration set (configset) that overrides the active configuration set attached to the model (modelObj). After the command is executed this override does not exist; the configuration set that is defined as 'active' is reinstated. To get the configuration sets attached to a model, use getconfigset. To attach a new or existing configuration set to a model, use addconfigset. To set the active configuration set of a model, use setactiveconfigset. For more information about configuration sets, see Configset object.  = sbiosimulate(modelObj, variantObj) simulates a model object (modelObj), using the variant object or array of variant objects (variantObj).</pre>		
	a model object (	ulate(modelObj, configsetObj, variantObj) simulates (modelObj), using the configuration set object and the variant object or array of variant objects	

# sbiosimulate

Property Summary	Configuration set property summary		
Johnnary	Active	Indicate object in use during simulation	
	CompileOptions	Dimensional analysis and unit conversion options	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	
	RuntimeOptions	Options for logged species	
	SensitivityAnalysisOptions	Specify sensitivity analysis options	
	SolverOptions	Specify model solver options	
	SolverType	Select solver type for simulation	
	StopTime	Set stop time for simulation	
	StopTimeType	Specify type of stop time for simulation	
	TimeUnits	Show stop time units for simulation	
	Туре	Display top-level SimBiology object type	
Examples	The following examples show how to change solver settings.		
	Example 1		
	<pre>Create a SimBiology model from an SBML file, simulate the mode using a solver other than the default solver (default is ode15s), an view the results. 1 Read the file for the oscillator model. modelObj = sbmlimport('oscillator.xml');</pre>		

**2** Get the active configset.

```
configsetObj = getconfigset(modelObj, 'active');
```

**3** Configure the SolverType to ode45 and set StopTime to 10.

```
set(configsetObj, 'SolverType', 'ode23s');
set(configsetObj, 'StopTime', 10);
```

**4** Simulate the modelObj.

[t,x]= sbiosimulate(modelObj);

**5** Plot the results of the simulation.

plot(t, x)

#### Example 2

Simulate the above example with DimensionalAnalysis off (set to false).

1 Repeat steps 1 and 2 above, then set dimensional analysis and unit conversion off in the configset object. DimensionalAnalysis and UnitConversion are properties of the CompileOptions object in the configset object.

```
set(configsetObj.CompileOptions, 'UnitConversion', false);
set(configsetObj.CompileOptions, 'DimensionalAnalysis', false);
```

**2** Simulate the modelObj.

simDataObj = sbiosimulate(modelObj);

**3** Plot the results of the simulation.

```
plot(simDataObj.Time, simDataObj.Data);
legend(simDataObj.DataNames)
```

See Also addconfigset, sbiomodel

## sbiospecies

Purpose	Construct species object		
	<b>Note</b> sbiospecies has addspecies instead.	been removed and produces an error. Use	
Syntax		es('NameValue') es('NameValue'), InitialAmountValue) es('PropertyName', PropertyValue)	
Arguments	NameValue	Name for a species object. Enter a character string unique to the level of object creation. Species objects are identified by Name within ReactionRate and Rule property strings. You can use the function sbioselect to find an object with a specific Name property value. For information on naming species, see Name.	
	InitialAmountValue	Initial amount value for the species object. Enter double. Positive real number, default = 0.	
Description	<pre>speciesObj = sbiospecies('NameValue') constructs a SimBiology.Species object, enters a value (NameValue) for the property Name, and returns the object (speciesObj).</pre>		
	<pre>speciesObj = sbiospecies('NameValue'), InitialAmountValue) in addition to the above, assigns an initial amount (InitialAmountValue) for the species.</pre>		
	-	t take part in reactions. A species object s. There are reserved characters you cannot use ne ( <i>NameValue</i> ).	
	_	ject to be used in a simulation, you must add SimBiology model object using copyobj. You	

can use addspecies to simultaneously create a species object and add it to a compartment object. A compartment object is constructed with the function addcompartment.

speciesObj = sbiospecies(...'PropertyName', PropertyValue...)
defines optional properties. The property name/property value pairs
can be in any format supported by the function set (for example,
name-value string pairs, structures, and name-value cell array pairs).

View species object properties with the function get, and change properties with the function set. You can find help for speciesObj properties with the help *PropertyName* command and help for functions with the sbiohelp *FunctionName* command.

A species is a chemical or entity that participates in reactions, for example, DNA, ATP, Pi, creatine, G-Protein, or Mitogen-Activated Protein Kinase (MAPK). Species amounts can vary or remain constant during a simulation.

If you change the Name property of a species you must configure all applicable elements, such as rules that use the species, any user-specified ReactionRate, or the kinetic law object property SpeciesVariableNames. Use the method setspecies to configure SpeciesVariableNames.

To update species names in the SimBiology graphical user interface, access each appropriate pane through the **Project Explorer**. You can also use the **Find** feature to locate the names that you want to update. The **Output** pane opens with the results of **Find**. Double-click a result row to go to the location of the model component.

Species names are automatically updated for reactions that use the MassAction kinetic law. See Name for more information about specifying species names.

## sbiospecies

Method Summary	Methods for species objects			
Sommary	copyobj (any object)	Copy SimBiology object and its children		
	delete (any object)	Delete SimBiology object		
	display (any object)	Display summary of SimBiology object		
	get (any object)	Get object properties		
	rename (compartment, parameter, species)	Rename object and update expressions		
	set (any object)	Set object properties		
Property Summary	Properties for species object			
	Annotation	Store link to URL or file		
	BoundaryCondition	Indicate species boundary condition		
	ConstantAmount	Specify variable or constant species amount		
	InitialAmount	Species initial amount		
	InitialAmountUnits	Species initial amount units		
	Name	Specify name of object		
	Notes	HTML text describing SimBiology object		
	Parent	Indicate parent object		
	Тад	Specify label for SimBiology object		

```
Display top-level SimBiology
                    Туре
                                                     object type
                    UserData
                                                     Specify data to associate with
                                                     object
Examples
                   Example 1
                   Create a species (H2O) and view properties for the object.
                   1 Create a species object named H20 and an initial amount of 1000.
                        speciesObj = sbiospecies('H2O', 1000);
                        % View the help for the species object's InitialAmount property.
                        help(speciesObj, 'InitialAmount')
                   2 View properties for the species object.
                         get(speciesObj)
                                     Annotation: ''
                             BoundaryCondition: 0
                                 ConstantAmount: 0
                                  InitialAmount: 1000
                            InitialAmountUnits: ''
                                           Name: 'H2O'
                                          Notes: ''
                                         Parent: []
                                            Tag: ''
```

#### Example 2

Create two species: one is a reactant and the other is the enzyme catalyzing the reaction.

UserData: []

Type: 'species'

 Create two species objects named glucose\_6\_phosphate and glucose\_6\_phosphate\_dehydrogenase.

### sbiospecies

speciesObj1 = sbiospecies ('glucose\_6\_phosphate'); speciesObj2 = sbiospecies ('glucose\_6\_phosphate\_dehydrogenase'); 2 Set the initial amount of glucose\_6\_phosphate to 100 and verify. set(speciesObj1, 'InitialAmount', 100); get(speciesObj1, 'InitialAmount') MATLAB returns: ans = 100 See Also addspecies MATLAB functions get, set

Purpose	Plot simulation results in subplots	
Syntax	yArgsValue)	fcnHandleValue, xArgsValue, fcnHandleValue, xArgsValue, ndValue)
Arguments	simDataObj fcnHandleValue xArgsValue yArgsValue showLegendValue	SimBiology data object. Function handle. Cell array with the names of the states. Cell array with the names of the states. Boolean (default is false).
Description	<pre>sbiosubplot(simDataObj) plots each simulation run for SimBiology data object, simDataObj into its own subplot. The subplot is a time plot of each state in simDataObj. A legend is included. sbiosubplot(simDataObj, fcnHandleValue, xArgsValue, yArgsValue) plots each simulation run for the SimBiology data object, simDataObj, into its own subplot. The subplot is plotted by calling the function handle, fcnHandleValue, with input arguments simDataObj, xArgsValue, and yArgsValue. sbiosubplot(simDataObj, fcnHandleValue, xArgsValue, yArgsValue, showLegendValue) plots each simulation run for the SimBiology data</pre>	
Examples	calling the function hand simDataObj, xArgsValue, if a legend is shown in the false. By default, showLeg	ts own subplot. The subplot is plotted by le, fcnHandleValue, with input arguments , and yArgsValue. showLegendValue indicates e plot. showLegendValue can be either true or gendValue is false. to plot data from an ensemble run without

```
% Load the radiodecay model.
    sbioloadproject('radiodecay.sbproj','m1');
    % Configure the model to run with the stochastic solver.
    cs = getconfigset(m1, 'active');
    set(cs, 'SolverType', 'ssa');
    set(cs.SolverOptions, 'LogDecimation', 100);
    % Run an ensemble simulation and view the results.
    simDataObj = sbioensemblerun(m1, 10, 'linear');
    sbiosubplot(simDataObj);
```



#### **Purpose** Create user-defined unit

```
Syntax unitObject = sbiounit('NameValue')
unitObject = sbiounit('NameValue', 'CompositionValue')
unitObject = sbiounit('NameValue', 'CompositionValue',
MultiplierValue)
unitObject = sbiounit('NameValue', 'CompositionValue',
MultiplierValue,OffsetValue)
unitObject = sbiounit('NameValue', 'CompositionValue',
...'PropertyName', PropertyValue...)
```

#### **Arguments**

NameValue	Name of the user-defined unit. <i>NameValue</i> must begin with characters and can contain characters, underscores, or numbers. <i>NameValue</i> can be any valid MATLAB variable name.
CompositionValue	Shows the combination of base and derived units that defines the unit <i>NameValue</i> . For example molarity is mole/liter. Base units are the set of units used to define all unit quantity equations. Derived units are defined using base units or mixtures of base and derived units.
MultiplierValue	Numerical value that defines the relationship between the user-defined unit <i>NameValue</i> and the base unit as a product of the <i>MultiplierValue</i> and the base unit. For example, 1 mole is 6.0221e23*molecule. The <i>MultiplierValue</i> is 6.0221e23.
OffsetValue	Numerical value by which the unit composition is modified. For example, Celsius = (5/9)*( Fahrenheit-32); Fahrenheit is Composition; <i>MultiplierValue</i> is 5/9 and <i>OffsetValue</i> is 32.

## sbiounit

	PropertyName	Name of the unit object property, for example, 'Notes'.	
	PropertyValue	Value of the unit object property, for example, 'New unit for GPCR model'.	
Description	object named NameVal	it(' <i>NameValue</i> ') constructs a SimBiology unit <i>lue</i> . Valid names must begin with a letter, and be nderscores, or numbers.	
	<pre>unitObject = sbiounit('NameValue', 'CompositionValue') allows you to specify the name and the composition of the unit.</pre>		
	unit with the name N	unitObject = sbiounit('NameValue','CompositionValue',MultiplierValue) creates a unit with the name NameValue where the unit is defined as MultiplierValue*CompositionValue.	
<pre>unitObject = sbiounit('NameValue','Compo creates a unit with the specifi</pre>		,'CompositionValue',MultiplierValue,OffsetValue) e specified offset.	
	<pre>unitObject = sbiounit('NameValue','CompositionValue','PropertyName', PropertyValue) defines optional properties. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).</pre>		
	with the sbioaddtol:	<i>bject</i> , you must add it to the user-defined library ibrary function. To get the unit object into the use the following command:	
	sbioaddtolibrary(	unitObject);	
		nal <i>unitObject</i> properties with the get command.	

You can view additional *unitObject* properties with the get command. You can modify additional properties with the set command. For more information about unit object properties and methods, see Unit object. Use the sbiowhos function to list the units available in the user-defined library.

**Examples** This example shows you how to create a user-defined unit, add it to the user-defined library, and query the library.

**1** Create units for the rate constants of a first-order and a second-order reaction.

```
unitObj1 = sbiounit('firstconstant', '1/second', 1);
unitObj2 = sbiounit('secondconstant', '1/molarity*second', 1);
```

2 Add the unit to the user-defined library.

sbioaddtolibrary(unitObj1); sbioaddtolibrary(unitObj2);

**3** Query the user-defined library in the root object.

rootObj = sbioroot; rootObj.UserDefinedLibrary.Units SimBiology UserDefined Units

Index:	Name:	Composition:	Multiplier:	Offset:
1	firstconstant	1/second	1.000000	0.000000
2	secondconstant	1/molarity*second	1.000000	0.000000

Alternatively, use the sbiowhos command.

sbiowhos -userdefined -unit

SimBiology UserDefined Units

## sbiounit

	Index:	Name:	Composition:	Multiplier:	Offset:
	1	firstconstant	1/second	1.000000	0.000000
	2	secondconstant	1/molarity*second	1.000000	0.000000
See Also	sbioaddtol	ibrary, sbiosh	owunits, sbiounitp	orefix, sbiowh	os

Purpose	Convert value between units
Syntax	<pre>result = sbiounitcalculator('fromUnits', 'toUnits', Value)</pre>
Description	<pre>result = sbiounitcalculator('fromUnits', 'toUnits', Value) converts the value, Value, which is defined in the units, fromUnits, to the value, result, which is defined in the units, toUnits.</pre>
Example	result = sbiounitcalculator('mile/hour','meter/second',1)
See Also	sbioshowunits

## sbiounitprefix

Purpose	Create user-defined unit prefix	
Syntax	<pre>unitprefixObject = sbiounitprefix('NameValue') unitprefixObject = sbiounitprefix('NameValue',     'ExponentValue') unitprefixObject = sbiounitprefix('NameValue',    'PropertyName', PropertyValue)</pre>	
Arguments	NameValue	Name of the user-defined unit prefix. <i>NameValue</i> must begin with characters and can contain characters, underscores, or numbers. <i>NameValue</i> can be any valid MATLAB variable name.
	ExponentValue	Shows the value of 10 <sup>Exponent</sup> that defines the relationship of the unit <i>Name</i> to the base unit. For example, for the unit picomole, Exponent is 12.
	PropertyName	Name of the unit prefix object property. For example, 'Notes'.
	PropertyValue	Value of the unit prefix object property. For example, 'New unitprefix for GPCR model'.
Description	<i>unitprefixObject</i> = sbiounitprefix(' <i>NameValue</i> ') constructs a SimBiology unit prefix object with the name <i>NameValue</i> . Valid names must begin with a letter, and be followed by letters, underscores, or numbers.	
		<pre>= sbiounitprefix('NameValue', 'ExponentValue') efix object with a multiplicative factor of ue'.</pre>
	PropertyValue name/property va	<pre>= sbiounitprefix('NameValue','PropertyName' .) defines optional properties. The property lue pairs can be in any format supported by the example, name-value string pairs, structures, and rray pairs).</pre>

,

	<pre>In order to use unitprefixObject, you must add it to the user-defined library with the sbioaddtolibrary function. To get the unit-prefix object into the user-defined library, use the following command: sbioaddtolibrary(unitprefixObject);</pre>
	You can view additional <i>unitprefixObject</i> properties with the get command. You can modify additional properties with the set command.
	Use the sbioshowunitprefixes function to list the units available in the user-defined library.
Examples	This example shows how to create a user-defined unit prefix, add it to the user-defined library, and query the library.
	1 Create a unit prefix.
	unitprefixObj1 = sbiounitprefix('peta', 15);
	<b>2</b> Add the unit prefix to the user-defined library.
	<pre>sbioaddtolibrary(unitprefixObj1);</pre>
	<b>3</b> Query the user-defined library in the root object.
	rootObj = sbioroot;
	rootObj.UserDefinedLibrary.UnitPrefixes
	Unit Prefix Array
	Index: Library: Name: Exponent:
	1 UserDefined peta 15
	Alternatively use the objection of a

Alternatively, use the sbiowhos command.

sbiowhos -userdefined -unitprefix

SimBiology UserDefined Unit Prefixes

Index: Name: Multiplier: 1 peta 1.000000e+015

**See Also** sbioaddtolibrary, sbioshowunits, sbiounit, sbiowhos

Purpose	Remove user-defined unit from root and library           Note         sbiounregisterunit has been removed and produces an error.           Use         sbioremovefromlibrary instead.
Syntax	<pre>sbiounregisterunit('Name')</pre>
Description	sbiounregisterunit('Name') removes the user-defined unit with the name Name from the user-defined library. You cannot remove a unit from the built-in library. If Name is a user-defined unit, then it is removed from the UserDefinedUnits vector on the SimBiology root object and also from the user library. Once unregistered, this unit is not available in future MATLAB sessions. You can list the available units and find information on whether the unit is built in or user defined using sbiowhos or sbioshowunits.
See Also	sbioremovefromlibrary, sbioshowunits, sbiounit, sbiowhos

Purpose	Remove user-defined unit prefix from root and library	
	<b>Note</b> sbiounregisterunitprefix has been removed and produces an error. Use sbioremovefromlibrary instead.	
Syntax	<pre>sbiounregisterunitprefix('Name')</pre>	
Description	sbiounregisterunitprefix('Name') removes the user-defined unit prefix with the name Name from the user-defined library. You cannot remove a unit prefix from the built-in library. If Name is a user-defined unit prefix, it is removed from the UserDefinedUnits vector on the SimBiology root object and also from the user library. Once unregistered, this unit prefix is not available in future MATLAB sessions. You can list the available unit prefixes and find information on whether the unit prefix is built in or user defined using sbiowhos or sbioshowunitprefixes.	
See Also	sbioremovefromlibrary, sbioroot, sbioshowunitprefixes, sbiounitprefix, sbiowhos	

Purpose	Update SimBiology model version		
Syntax	<i>modelsObj</i> = sbioupdate( <i>modelObj</i> ) <i>simdataObj</i> = sbioupdate( <i>tsObj</i> )		
Arguments	modelsObj	sbioupdate output. Contains an array of model objects that includes the top-level model object and a model object for each previously existing submodel.	
	mode10bj	Model object with submodels to be converted into separate model objects.	
	simdataObj	sbioupdate output. Contains a SimData object converted from previous time series object.	
	tsObj	Time series object to be converted to a SimData object. Can be a 1-by-n cell array of time series objects.	
Description	<ul> <li>modelsObj = sbioupdate(modelObj) converts a top level SimBiology model object (modelObj) that has submodels into an array of SimBiology model objects which do not have any submodels.</li> <li>There is one model for the top model and one for each of the submodels. Each model created, has a copy of all the parameters used by the model, including those that belonged to the parent model. Updating deletes any unused parameters in the parent model.</li> </ul>		
	Each model created from the previously existing submodel has empty StatesToLog, SpeciesInputFactors, ParameterInputFactors, and SpeciesOutputs property values.		
	<pre>simdataObj = sbioupdate(tsObj) converts a time series object (tsObj) obtained from simulation of a SimBiology model into a SimData object. If tsObj is a cell array of time series objects, then simdataObj is an array of SimData objects, having one element for each of the time series objects in tsObj.</pre>		

## sbiovariant

Purpose	Construct variant object		
Syntax	<pre>variantObj = sbiovariant('NameValue') variantObj = sbiovariant('NameValue', 'ContentValue') variantObj = sbiovariant('PropertyName', PropertyValue)</pre>		
Arguments	modelObj	Specify the model object to which you want add a variant.	
	variant0bj	Variant object to create and add to the model object.	
	NameValue	Name of the variant object. <i>NameValue</i> is assigned to the Name property of the variant object.	
Description	<pre>variantObj = sbiovariant('NameValue') creates a SimBiology variant object (variantObj) with the name NameValue. The variant object Parent property is assigned [] (empty).</pre>		
	<pre>variantObj = sbiovariant('NameValue', 'ContentValue') creates a SimBiology variant object (variantObj) with the Content property set to ContentValue.</pre>		
	To add a variant to a model use the copyobj method. A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see Variant object.		
	<pre>variantObj = sbiovariant('PropertyName', PropertyValue) defines optional properties. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).</pre>		
		variant object with the get command, and modify at object with the set command.	

**Note** Remember to use the addcontent method instead of using the set method on the Content property because the set method replaces the data in the Content property, whereas addcontent appends the data.

Method Summary	addcontent (variant) commit (variant) copyobj (any object)	Append content to variant object Commit variant contents to model Copy SimBiology object and its children
	delete (any object) display (any object)	Delete SimBiology object Display summary of SimBiology object
	get (any object)	Get object properties
	rmcontent (variant)	Remove contents from variant object
	set (any object)	Set object properties
	verify (model, variant)	Validate and verify SimBiology model
Property Summary	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	Content	Contents of variant object
	Name	Specify name of object
	Notes	HTML text describing SimBiology object

	Parent	Indicate parent object
	Tag	Specify label for SimBiology object
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object
Examples	<pre>l Create a variant object. variantObj = sbiovariant('p1');</pre>	
	<b>2</b> Add content to the variant object that varies the InitialAmount property of a species named A.	
	addcontent(variantObj, {'	<pre>species', 'A', 'InitialAmount', 5});</pre>
See Also	addvariant, copyobj, getvariant	

**Purpose** Show contents of project file, library file, or SimBiology root object

#### Syntax sbiowhos flag sbiowhos ('flag') sbiowhos flag1 flag2... sbiowhos FileName

**Description** sbiowhos shows contents of the SimBiology root object. This includes the built-in and user-defined abstract kinetic laws, units, and unit prefixes.

sbiowhos flag shows specific information about the SimBiology root object as defined by flag. Valid flags are described in this table.

Flag	Description
-builtin	Built-in abstract kinetic laws, units, and unit prefixes
-data	Data saved in file
-kineticlaw	Built-in and user-defined abstract kinetic laws
-unit	Built-in and user-defined units
-unitprefix	Built-in and user-defined unit prefixes
-userdefined	User-defined abstract kinetic laws, units, and unit prefixes

You can also specify the functional form sbiowhos ('flag').

sbiowhos *flag1 flag2...* shows information about the SimBiology root object as defined by *flag1*, *flag2,...*.

sbiowhos *FileName* shows the contents of the SimBiology project or library defined by Name.

## sbiowhos

Examples	% Show contents of the SimBiology root object sbiowhos	
	% Show abstract kinetic laws on the SimBiology root object sbiowhos -kineticlaw	
	% Show the builtin units of the SimBiology root object. sbiowhos -builtin -unit	
	% Show all contents of project file. sbiowhos myprojectfile	
	% Show abstract kinetic laws from a library file. sbiowhos -kineticlaw mylibraryfile	
	% Show all contents of multiple files. sbiowhos myfile1 myfile2	
See Also	MATLAB function whos	

Purpose	Export SimBiology model to SBML file			
Syntax		<pre>sbmlexport(modelObj) sbmlexport(modelObj, 'FileName')</pre>		
Arguments	modelObj FileName	Model object. Enter a variable name for a model object. XML file with a Systems Biology Markup Language (SBML) format. Enter either a file name or a path and file name supported by your operating system. If the file name does not have the extension .xml, then .xml is appended to end of the file name.		
Description	<pre>sbmlexport(modelObj) exports a SimBiology model object (modelObj) to a file with a Systems Biology Markup Language (SBML) Level 2 Version 1 format. The default file extension is .xml and the file name matches the model name. sbmlexport(modelObj, 'FileName') exports a SimBiology model object (modelObj) to an SBML file named FileName. The default file extension is .xml.</pre>			
	A SimBiology model can also be written to a SimBiology project with the sbiosaveproject function to save features not supported by SBML.			
	See "SBML Support" in the SimBiology Getting Started Guide for more information.			
Example	Export a model (modelObj) to a file (gene_regulation.xml) in the current working directory.			
	sbmlexport	t(modelObj,'gene_regulation.xml');		
Reference	Finney, A., Hucka, M., (2003), Systems Biology Markup Language (SBML) Level 2: Structures and facilities for model definitions. Accessed from SBML.org			

See Also sbiomodel, sbiosaveproject, sbmlimport

## sbmlimp<u>ort</u>

Purpose	Import SBML-formatted file		
Syntax	<pre>modelObj = sbmlimport('FileName')</pre>		
Arguments	<b>FileName</b> XML file with a Systems Biology Markup Language (SBML) format. Enter either a file name or a path and file name supported by your operating system.		
Description	<pre>modelObj = sbmlimport('FileName') imports an SBML-formatted file with name FileName into MATLAB and creates a model object modelObj. FileName extensions can be .sbml or .xml. The modelObj properties can be viewed with the get command. modelObj properties can be modified with the set command. At the command line, help for modelObj functions can be returned with the sbiohelp command. sbmlimport supports SBML Levels 1 and Level 2 Version 1.</pre>		
	See "SBML Support" in the SimBiology Getting Started Guide for more information.		
Example	<pre>sbmlobj = sbmlimport('oscillator.xml');</pre>		
Reference	Finney, A., Hucka, M., (2003), Systems Biology Markup Language (SBML) Level 2: Structures and facilities for model definitions. Accessed from SBML.org.		
See Also	get, sbmlexport, sbiosimulate, set		

## sbmlimport

# Method Reference

Objects (p. 3-2)	SimBiology objects
	Work with abstract kinetic law
Abstract Kinetic Laws (p. 3-2)	objects
Compartments (p. 3-3)	Work with compartment objects
Configuration Sets (p. 3-4)	Work with configuration set objects
Events (p. 3-4)	Work with event objects
Kinetic Laws (p. 3-5)	Create parameter objects and work with kinetic law objects
Models (p. 3-6)	Create SimBiology objects and work with model objects
Parameters (p. 3-8)	Work with parameter objects
Reactions (p. 3-9)	Create kinetic law and species objects and work with reaction objects
Root (p. 3-10)	Work with the root object
Rules (p. 3-11)	Work with rule objects
SimData (p. 3-12)	Methods for SimData objects
Species (p. 3-13)	Methods for species objects
Units and Unit Prefixes (p. 3-13)	Methods for unit and prefix objects
Variants (p. 3-13)	Methods for variant objects
Using Object Methods (p. 3-15)	Command-line syntax for using methods with SimBiology objects

### Objects

AbstractKineticLaw object Compartment object Configset object Event object KineticLaw object Model object

Parameter object Reaction object

Root object

Rule object SimData object Species object Unit object

UnitPrefix object

Variant object

Kinetic law information in library Options for compartments Solver settings information for model simulation Store event information Kinetic law information for reaction Model and component information Parameter and scope information Options for model reactions Hold models, unit libraries, and abstract kinetic law libraries Hold rule for species and parameters Simulation data storage Options for compartment species Hold information about user-defined unit Hold information about user-defined unit prefix

Store alternate component values

### **Abstract Kinetic Laws**

delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
set (any object)	Set object properties

## Compartments

addcompartment (model, compartment)	Create compartment object
addspecies (compartment)	Create species object and add to compartment object
copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
rename (compartment, parameter, species)	Rename object and update expressions
reorder (model, compartment)	Reorder component lists
set (any object)	Set object properties

## **Configuration Sets**

copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
set (any object)	Set object properties

#### **Events**

copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
set (any object)	Set object properties

## **Kinetic Laws**

addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
getparameters (kineticlaw)	Get specific parameters in kinetic law object
getspecies (kineticlaw)	Get specific species in kinetic law object
set (any object)	Set object properties
setparameter (kineticlaw)	Specify specific parameters in kinetic law object
setspecies (kineticlaw)	Specify species in kinetic law object

## **Models**

addcompartment (model, compartment)	Create compartment object
addconfigset (model)	Create configuration set object and add to model object
addevent (model)	Add event object to model object
addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
addreaction (model)	Create reaction object and add to model object
addrule (model)	Create rule object and add to model object
addvariant (model)	Add variant to model
copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
getadjacencymatrix (model)	Get adjacency matrix from model object
getconfigset (model)	Get configuration set object from model object
getstoichmatrix (model)	Get stoichiometry matrix from model object
getvariant (model)	Get variant from model
removeconfigset (model)	Remove configuration set from model
removevariant (model)	Remove variant from model
reorder (model, compartment)	Reorder component lists
set (any object)	Set object properties

setactiveconfigset (model)	Set active configuration set for model object
verify (model, variant)	Validate and verify SimBiology model

### **Parameters**

copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
rename (compartment, parameter, species)	Rename object and update expressions
set (any object)	Set object properties

### Reactions

addkineticlaw (reaction)	Create kinetic law object and add to reaction object
addproduct (reaction)	Add product species object to reaction object
addreactant (reaction)	Add species object as reactant to reaction object
copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants
set (any object)	Set object properties

### Root

copyobj (any object)	Copy SimBiology object and its children
get (any object)	Get object properties
reset (root)	Delete all model objects from root object
set (any object)	Set object properties

## Rules

copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
set (any object)	Set object properties

### SimData

delete (any object) Delete SimBiology object display (any object) Display summary of SimBiology object get (any object) Get object properties getdata (SimData) Get data from SimData object array getsensmatrix (SimData) Get 3-D sensitivity matrix from SimData array Resample SimData object array onto resample (SimData) new time vector select (SimData) Select data from SimData object selectbyname (SimData) Select data by name from SimData object array

## **Species**

copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
rename (compartment, parameter, species)	Rename object and update expressions
set (any object)	Set object properties

## **Units and Unit Prefixes**

delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
set (any object)	Set object properties

### Variants

addcontent (variant)	Append content to variant object
commit (variant)	Commit variant contents to model
copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object

display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
rmcontent (variant)	Remove contents from variant object
set (any object)	Set object properties
verify (model, variant)	Validate and verify SimBiology model

### **Using Object Methods**

Command-line syntax for using methods with SimBiology objects

Constructing (Creating) Objects (p. 3-15)

Using Object Methods (p. 3-15)

Help for Objects, Methods, and Properties (p. 3-16)

### **Constructing (Creating) Objects**

Create an object that is not referenced by a model using the constructor functions sbioabstractkineticlaw, sbiomodel, sbioparameter, sbioreaction, sbioroot, sbiorule, and sbiospecies.

```
To create objects referenced by a model, use the model object methods addconfigset, addmodel, addparameter, addreaction, addrule, and addspecies.
```

ObjectName = ModelName.Method(Arguments)

To create objects referenced by a reaction, use the reaction object methods addkineticlaw, addparameter, addproduct, and addreactant.

ObjectName = ReactionName.Method(Arguments)

Note that ObjectName is not a copy of the object, but a pointer to the created object.

### **Using Object Methods**

Using MATLAB function notation:

```
MethodName(ObjectName, arguments, ...)
```

Using object dot notation:

ObjectName.MethodName(arguments, ...)

### Help for Objects, Methods, and Properties

Display information for SimBiology object methods and properties in the MATLAB Command Window.

help sbio	Display a list of functions and methods.
help FunctionName	Display function information.
<pre>sbiohelp('MethodName')</pre>	Display method information.
<pre>sbiohelp('PropertyName')</pre>	Display property information.

# Methods — Alphabetical List

The object that the methods apply to are listed in parenthesis after the method name.

#### **Purpose** Kinetic law information in library

**Description** The abstract kinetic law object represents an *abstract kinetic law*, which provides a mechanism for applying a rate law to multiple reactions. The information in this object acts as a mapping template for the reaction rate. The abstract kinetic law defines a mathematical relationship that defines the rate at which reactant species are produced and product species are consumed in the reaction. The expression is shown in the property Expression. The species variables are defined in the SpeciesVariables property, and the parameter variables are defined in the ParameterVariables property of the abstract kinetic law object. For an explanation of how the abstract kinetic law object.

Define your own abstract kinetic law and add it to the abstract kinetic law library with the sbioaddtolibrary function. You can then use the abstract kinetic law when constructing a kinetic law object with the method addkineticlaw. To retrieve an abstract kinetic law object from the user-defined library, use the command get(sbioroot, 'UserDefinedKineticLaws').

See "Property Summary" on page 4-3 for links to abstract kinetic law object property reference pages.

Properties define the characteristics of an object. For example, an abstract kinetic law object includes properties for the expression, the name of the law, parameter variables, and species variables. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the SimBiology desktop.

#### Constructor Summary

sbioabstractkineticlaw

Construct abstract kinetic law object

Method Summary	delete (any object) display (any object) get (any object) set (any object)	Delete SimBiology object Display summary of SimBiology object Get object properties Set object properties	
Property Summary	Annotation Expression	Store link to URL or file Expression to determine reaction rate equation	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	
	ParameterVariables	Parameters in abstract kinetic law	
	Parent	Indicate parent object	
	SpeciesVariables	Species in abstract kinetic law	
	Тад	Specify label for SimBiology object	
	Туре	Display top-level SimBiology object type	
	UserData	Specify data to associate with object	
See Also	Configset object, KineticLaw o object, Reaction object, Root o		

object

## addcompartment (model, compartment)

Purpose	Create compartment object			
Syntax	<pre>compartmentObj = addcompartment(modelObj, 'NameValue') compartmentObj = addcompartment(owningCompObj, 'NameValue') compartmentObj = addcompartment(modelObj, 'NameValue',     CapacityValue) compartmentObj = addcompartment('PropertyName', PropertyValue)</pre>			
Arguments	modelObj owningCompObj	Model object. Compartment object that contains the newly created compartment object.		
	NameValue	Name for a compartment object. Enter a character string unique to the model object. For information on naming compartments, see Name.		
	CapacityValue Capacity value for the compartment objec Enter double. Positive real number, defau = 1.			
	PropertyName	Enter the name of a valid property. Valid property names are listed in "Property Summary" on page 4-6.		
	PropertyValue	Enter the value for the property specified in <i>PropertyName</i> . Valid property values are listed on each property reference page.		
Description	<pre>compartmentObj = addcompartment(modelObj, 'NameValue') creates a compartment object and returns the compartment object (compartmentObj). In the compartment object, this method assigns a value (NameValue) to the property Name, and assigns the model object</pre>			

(modelObj) to the property Parent. In the model object, this method assigns the compartment object to the property Compartments.

compartmentObj = addcompartment(owningCompObj, 'NameValue') in addition to the above, adds the newly created compartment within a compartment object (owningCompObj), and assigns this compartment object (owningCompObj) to the Owner property of the newly created compartment object (compartmentObj). The parent model is the model that contains the owning compartment (owningCompObj).

compartmentObj = addcompartment(modelObj, 'NameValue', CapacityValue), in addition to the above, this method assigns capacity (CapacityValue) for the compartment.

If you define a reaction within a model object (modelObj) that does not contain any compartments, the process of adding a reaction generates a default compartment object and assigns the reaction species to the compartment. If there is more than one compartment, you must specify which compartment the species should be assigned to using the format *CompartmentName.SpeciesName*.

View properties for a compartment object with the get command, and modify properties for a compartment object with the set command. You can view a summary table of compartment objects in a model (modelObj) with get(modelObj, 'Compartments') or the properties of the first compartment with get(modelObj.Compartments(1)).

compartmentObj = addcompartment(...'PropertyName', PropertyValue...) defines optional properties. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs). "Property Summary" on page 4-6 lists the properties. The Owner property is one exception; you cannot set the Owner property in the addcompartment syntax because, addcompartment requires the owning model or compartment to be specified as the first argument and uses this information to set the Owner property. After adding a compartment, you can change the owner using the function set.

## addcompartment (model, compartment)

Method Summary	Methods for compartment objects addcompartment (model, Create compartment object compartment)			
	addspecies (compartment)	Create species object and add to compartment object		
	copyobj (any object)	Copy SimBiology object and its children		
	delete (any object)	Delete SimBiology object		
	display (any object)	Display summary of SimBiology object		
	get (any object)	Get object properties		
	rename (compartment, parameter, species)	Rename object and update expressions		
	reorder (model, compartment)	Reorder component lists		
	set (any object)	Set object properties		
Property Summary	Properties for compartment objects	S		
Joinnai y	Annotation	Store link to URL or file		
	Capacity	Compartment capacity		
	CapacityUnits	Compartment capacity units		
	Compartments	Array of compartments in model or compartment		
	ConstantCapacity	Specify variable or constant compartment capacity		
	Name	Specify name of object		
	Notes	HTML text describing SimBiology object		

Owner		(	Owning compartment	
	Parent	]	Indicate parent object	
	Species		Array of species in compartment object	
	Tag		Specify label for SimBiology object	
	Туре		Display top-level SimBiology object type	
	UserData		Specify data to as object	ssociate with
Examples	1 Create a model	object (modelObj).		
	<pre>modelObj = sbiomodel('cell'); 2 Add two compartments to the model object.</pre>			
compartmentObj1 = addcompartmen compartmentObj2 = addcompartmen				
	<b>3</b> Add a compartment to one of the compartment objects.			ets.
	<pre>compartmentObj3 = addcompartment(compartmentObj2, 'matrix');</pre>			
	4 Display the Compartments property in the model object. get(modelObj, 'Compartments') SimBiology Compartment Array			ject.
	Index: 1 2 3	Name: nucleus mitochondrion matrix	Capacity: 1 1 1	CapacityUnits:

### addcompartment (model, compartment)

**5** Display the Compartments property in the compartment object.

```
get(compartmentObj2, 'Compartments')
SimBiology Compartment - matrix
Compartment Components:
   Capacity: 1
   CapacityUnits:
   Compartments: 0
   ConstantCapacity: true
   Owner: mitochondrion
   Species: 0
```

See Also addproduct, addreactant, addreaction, addspecies, get, set

Purpose	Create configuration set object and add to model object	
Syntax	configsetObj = addconfigset(modelObj, 'NameValue') configsetObj = addconfigset(, 'PropertyName', PropertyValue,)	
Arguments	model0bjModel object. Enter a variable name.NameValueDescriptive name for a configuration set object. Reserved words 'active' and 'default' are not allowed.configset0bjConfiguration set object.	
Description	<pre>configsetObj = addconfigset(modelObj, 'NameValue') creates a configuration set object and returns to configsetObj. In the configuration set object, this method assigns a value (NameValue) to the property Name. configsetObj = addconfigset(, 'PropertyName', PropertyValue, ) constructs a configuration set object, configsetObj, and configures configsetObj with property value pairs. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs). The configsetObj properties are listed in "Property Summary" on page 4-10. A configuration set stores simulation specific information. A model object can contain multiple configuration sets, with one being active at any given time. The active configuration set contains the settings that are used during a simulation. configsetObj is not automatically set to active. Use the function setactiveconfigset to define the active configset for modelObj. Use the method copyobj to copy a configset object and add it to the modelObj.</pre>	

	You can additionally view configurations command get. You can modify add properties with the command set.	
Method	Methods for configuration set object	ts
Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	set (any object)	Set object properties
Property Summary	Properties for configuration set objects	
Johnnary	Active	Indicate object in use during simulation
	CompileOptions	Dimensional analysis and unit conversion options
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	RuntimeOptions	Options for logged species

Specify sensitivity analysis

Specify model solver options

Set stop time for simulation

Specify type of stop time for

Select solver type for simulation

options

simulation

SensitivityAnalysisOptions

SolverOptions

StopTimeType

SolverType

StopTime

	TimeUnits	Show stop time units for simulation
	Туре	Display top-level SimBiology object type
Examples	<ol> <li>Create a model object by reading configuration set that simulates to</li> </ol>	the file oscillator.xml and add a the model for 3000 seconds.
	modelObj = sbmlimport('o configsetObj = addconfigs	
	2 Configure the configsetObj Sto	pTime to 3000.
	set(configsetObj, 'StopTin get(configsetObj)	me', 3000)
	Name: 'myse Notes: '' RuntimeOptions: [1x1 s	SimBiology.RuntimeOptions] SimBiology.ODESolverOptions] 5s' lationTime' nd'
	<b>3</b> Set the new configset to be actinew configset, and plot the rest	
	<pre>setactiveconfigset(model [t,x] = sbiosimulate(model plot (t,x)</pre>	
See Also	get, getconfigset, removeconfig	set, set, setactiveconfigset

## addcontent (variant)

Purpose	Append content to variant object	
Syntax	addcontent(variantObj, contents) addcontent(variantObj1, variantObj2)	
Arguments	variantObj	Specify the variant object to which you want to append data. The Content property is modified to add the new data.
	contents	Specify the data you want to add to a variant object. Contents can either be a cell array or an array of cell arrays. A valid cell array should have the form {'Type', 'Name', 'PropertyName', PropertyValue}, where PropertyValue is the new value to be applied for the PropertyName. Valid Type, Name, and PropertyName values are as follows.

′Туре′	'Name'	'PropertyName'
'species'	Name of the species. If there are multiple species in the model with the same name, specify the species as [compartmentName.speciesName], where compartmentName is the name of the compartment containing the species.	'InitialAmount'
'parameter'	If the parameter scope is a model, specify the parameter name. If the parameter scope is a kinetic law, specify [reactionName.parameterName].	'Value'
'compartment'	Name of the compartment.	'Capacity'

Description	addcontent( <i>variantObj</i> , <i>contents</i> ) adds the data stored in the variable
	contents to the variant object (variantObj).

addcontent(*variantObj1*, *variantObj2*) appends the data in the Content property of the variant object *variantObj2* to the Content property of variant object *variantObj1*.

**Note** Remember to use the addcontent method instead of using the set method on the Content property because the set method replaces the data in the Content property, whereas addcontent appends the data.

Examples	1 Create a model containing one species.		
<pre>modelObj = sbiomodel('mymodel'); compObj = addcompartment(modelObj, 'comp1'); speciesObj = addspecies(compObj, 'A');</pre>			
	<b>2</b> Add a variant object that varies the InitialAmount property of a species named A.		
	variantObj = addvariant(modelObj, 'v1'); addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});		
See Also	addvariant, rmcontent, sbiovariant		

### addevent (model)

Purpose	Add event object to model object	
Syntax	<pre>eventObj = addevent(modelObj, 'TriggerValue',     'EventFcnsValue') eventObj = addevent('PropertyName', PropertyValue)</pre>	
Arguments	mode10bjModel object.TriggerValueRequired property to specify a trigger condition.	
		Must be a MATLAB expression that evaluates to a logical value. Use the keyword 'time' to specify that an event occurs at a specific time during the simulation. See Trigger for more information.
	EventFcnsValue	A string or a cell array of strings, each of which specifies an assignment of the form 'objectname = expression', where objectname is the name of a valid object. Defines what occurs when the event is triggered. See EventFcns for more information.
	PropertyName	Property name for an event object from "Property Summary" on page 4-15.
	PropertyValue	Property value. For more information on property values, see the property reference for each property listed in "Property Summary" on page 4-15.
Description		

**Description** eventObj = addevent(modelObj, 'TriggerValue', 'EventFcnsValue') creates an event object (eventObj) and adds the event to the model (modelObj). In the event object, this method assigns a value (TriggerValue) to the property TriggerCondition, assigns a value (EventFcnsValue) to the property EventFcns, and assigns the model object (modelObj) to the property Parent. In the model object, this method appends the event object to the property Events.

	When the trigger expression in the property Trigger changes from false to true, the assignments in EventFcns are executed during simulation.		
	For details on how events are handled during a simulation, see "Changing Model Component Values Using Events" in the SimBiology User's Guide documentation.		
	eventObj = addevent(' <i>PropertyName</i> ', <i>PropertyValue</i> ) defines optional properties. The property name and property value pairs can be any format supported by the function <b>set</b> (for example, name-value string pairs, structures, and name-value cell array pairs).		
	You can view additional object properties with the get command. You can modify additional object properties with the set command. To view events of a model object (modelObj), use the command get(modelObj, 'Events').		
Method Summary	copyobj (any object)	Copy SimBiology object and its children	
	delete (any object)	Delete SimBiology object	
	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	
	set (any object)	Set object properties	
Property Summary	Active	Indicate object in use during simulation	
	Annotation	Store link to URL or file	
	EventFcns	Event expression	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	

	Parent	Indicate parent object
	Tag	Specify label for SimBiology object
	Trigger	Event trigger
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object
Examples	1 Create a model object, and	then add an event object.
	modelObj = sbmlimpor <sup>.</sup> eventObj = addevent(n	t('oscillator') modelObj, 'time>= 5', 'OpC = 200');
	<b>2</b> Get a list of properties for a	an event object.
	get(modelObj.Events(	1));
	Or	
	get(eventObj)	
	MATLAB displays a list of	event properties.
	Active:	
	Annotation:	1.1
	EventFcns:	{ 'OpC = 200 ' }
	Nalie.	1.1
	Notes:	
		[1x1 SimBiology.Model]
	Tag:	
		'time >= 5'
	Type:	'event'

UserData: []

See Also Event object

Purpose	Create kinetic law object and add to reaction object	
Syntax	<pre>kineticlawObj = addkineticlaw(reactionObj,</pre>	
Arguments	reactionObj	Reaction object. Enter a variable name for a reaction object.
	KineticLawNameValue	Property to select the type of kinetic law object to create. For built-in kinetic law, valid values are:
		'Unknown', 'MassAction', 'Henri-Michaelis-Menten', 'Henri-Michaelis-Menten-Reversible', 'Hill-Kinetics', 'Iso-Uni-Uni', 'Ordered-Bi-Bi', 'Ping-Pong-Bi-Bi', 'Competitive-Inhibition', 'NonCompetitive-Inhibition', and 'UnCompetitive-Inhibition'.
		Find valid <i>KineticLawNameValues</i> by querying the SimBiology root object with the commands get(sbioroot, 'BuiltInKineticLaws'), and get(sbioroot, 'UserDefinedKineticLaws').
		sbiowhos -kineticlaw lists BuiltInKineticLaws and UserDefinedKineticLaws in the SimBiology root. The root contains all BuiltInKineticLaws and all UserDefinedKineticLaws that are added using sbioaddtolibrary.

#### **Description** kineticlawObj = addkineticlaw(reactionObj, 'KineticLawNameValue') creates a kinetic law object and returns the kinetic law object (kineticlawObj).

In the kinetic law object, this method assigns a name (*KineticLawNameValue*) to the property KineticLawName and assigns the reaction object to the property Parent. In the reaction object, this method assigns the kinetic law object to the property KineticLaw.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'a -> b');
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
parameterObj = addparameter(kineticlawObj, 'K1_forward', 0.1);
set(kineticlawObj, ParameterVariableName, 'K1_forward');
```

modelObj
modelObj.Name = 'cell'
modelObj.Reactions(1)
/ mode/Obj.Reactions(1).Reaction = 'a -> b'
mode/Obj.Reactions(1).Parent = mode/Obj
modelObj.Reactions(1).KineticLaw(1)
mode/Obj.Reactions(1).Kinetid_aw.Type = 'MassAction' mode/Obj.Reactions(1).Kinetid_aw.Parent = reactionObj mode/Obj.Reactions(1).Kinetid_aw.Parameters = parameterObj
modelObj.Reactions(1).KineticLaw.Parameters(1)
mode/Obj.Reactions(1).Kinetid_aw.Parameters(1).Name = 'K1_forward' mode/Obj.Reactions(1).Kinetid_aw.Parameters(1).Value = 0.1 mode/Obj.Reactions(1).Kinetid_aw.Parameters(1).Parent = kinetidawObj

*KineticLawNameValue* is any valid abstract kinetic law. See "Abstract Kinetic Law" on page 6-49 for a definition of abstract kinetic laws and more information about how they are used to get the reaction rate expression.

	kineticlawObj= addkineticlaw(, 'PropertyName', PropertyN ) constructs a kinetic law object, kineticlawObj, and configu kineticlawObj with property value pairs. The property name/pr value pairs can be in any format supported by the function set ( example, name-value string pairs, structures, and name-value ca array pairs). The kineticlawObj properties are listed in "Prope Summary" on page 4-21.		
	You can view additional kinetic law object properties with the get command. You can modify additional kinetic law object properties with the set command. The kinetic law used to determine the ReactionRate of the Reaction can be viewed with get( <i>reactionObj</i> , 'KineticLaw'). Remove a SimBiology kinetic law object from a SimBiology reaction object with the delete command.		
Method	Methods for kinetic law objects		
Summary	addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object	
	copyobj (any object)	Copy SimBiology object and its children	
	delete (any object)	Delete SimBiology object	
	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	
	getparameters (kineticlaw)	Get specific parameters in kinetic law object	
	getspecies (kineticlaw)	Get specific species in kinetic law object	
	set (any object)	Set object properties	

## addkineticlaw (reaction)

	setparameter (kineticlaw)	Specify specific parameters in kinetic law object		
	setspecies (kineticlaw)	Specify species in kinetic law object		
Property Summary	Properties for kinetic law objects			
	Annotation	Store link to URL or file		
	Expression	Expression to determine reaction rate equation		
	KineticLawName	Name of kinetic law applied to reaction		
	Name	Specify name of object		
	Notes	HTML text describing SimBiology object		
	Parameters	Array of parameter objects		
	ParameterVariableNames	Cell array of reaction rate parameters		
	ParameterVariables	Parameters in abstract kinetic law		
	Parent	Indicate parent object		
	SpeciesVariableNames	Cell array of species used in reaction rate equation		
	SpeciesVariables	Species in abstract kinetic law		
	Tag	Specify label for SimBiology object		

Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

#### **Examples** Example 1

This example uses the built-in kinetic law Henri-Michaelis-Menten.

1 Create a model object, and add a reaction object to the model.

```
modelObj = sbiomodel ('Cell');
reactionObj = addreaction (modelObj, 'Substrate -> Product');
```

**2** Define an abstract kinetic law for the reaction object and view the parameters to be set.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
get (kineticlawObj, 'Expression')
```

```
ans =
Vm*S/(Km + S)
```

The addkineticlaw method adds an abstract kinetic law expression to the reaction object (*reactionObj*).

The Henri-Michaelis-Menten kinetic law has two parameters (Vm and Km) and one species (S). You need to enter values for these parameters by first creating parameter objects, and then adding the parameter objects to the kinetic law object.

**3** Add parameter objects to a kinetic law object. For example, create a parameter object parameterObj1 named Vm\_d, another parameter parameterObj2) named Km\_d, and add them to a kinetic law object (kineticlawObj).

```
parameterObj1 = addparameter(kineticlawObj, 'Vm_d', 'Value', 6.0);
parameterObj2 = addparameter(kineticlawObj, 'Km_d', 'Value', 1.25);
```

The addparameter method creates two parameter objects with concrete values that will be associated with the abstract kinetic law parameters.

**4** Associate concrete kinetic law parameters with the abstract kinetic law parameters.

```
set(kineticlawObj,'ParameterVariableNames', {'Vm_d' 'Km_d'});
set(kineticlawObj,'SpeciesVariableNames', {'Substrate'});
```

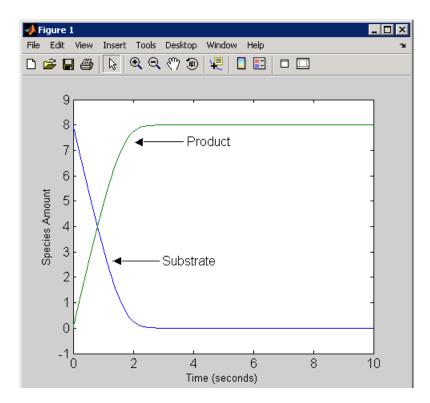
This method associates the concrete parameters in the property ParameterVariableNames with the abstract parameters in the property ParameterVariables using a one-to-one mapping in the order given.

**5** Verify that the reaction rate is expressed correctly in the reaction object ReactionRate property.

```
get (reactionObj, 'ReactionRate')
ans =
    Vm_d*Substrate/(Km_d+Substrate)
```

**6** Enter an initial value for the substrate and simulate.

```
modelObj.Species(1).InitialAmount = 8;
[T, X] = sbiosimulate(modelObj);
plot(T,X)
```



#### Example 2

This example uses the built-in kinetic law MassAction.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('Cell');
reactionObj = addreaction (modelObj, 'a -> b');
```

**2** Define an abstract kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
get(kineticlawObj, 'Expression')
ans =
```

MassAction

Notice, the property Expression for an abstract kinetic law with property Type set to MassAction does not show the parameters and species in the reaction rate.

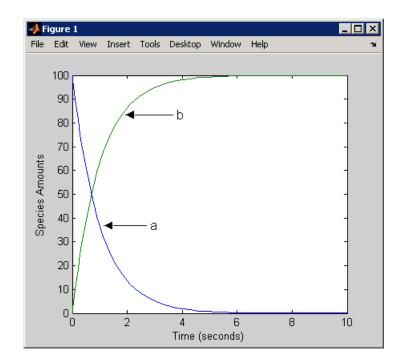
**3** Assign the rate constant for the reaction.

```
parameterObj = addparameter(kineticlawObj, 'k_forward');
set (kineticlawObj, 'ParameterVariablenames', 'k_forward');
get (reactionObj, 'ReactionRate')
ans =
    k_forward*a
```

**4** Enter an initial value for the substrate and simulate.

modelObj.Species(1).InitialAmount = 100; [T, X] = sbiosimulate(modelObj);plot(T,X)

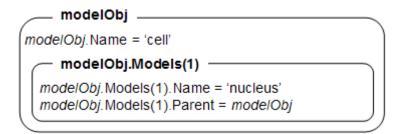
The value used for  $k_forward$  is the default value = 1.0.





addreaction, setparameter

Purpose	Add submodel object to model object			
	<b>Note</b> addmodel produces a warning and will be removed in a future version. Submodels will not be supported in future releases. Use the function sbioupdate to convert submodels into models.			
Syntax	<pre>submodelObj = addmodel(modelObj, 'NameValue') submodelObj = addmodel('PropertyName', PropertyValue)</pre>			
Arguments	modelObj NameValue SubmodelObj	Model object. Enter a name for a model object. Descriptive name for a model object. Enter a unique character string. A model object can be referenced by other objects using this property. Model object to be added as a submodel		
Description	<pre>submodelObj Model object to be added as a submodel. submodelObj = addmodel(modelObj, 'NameValue') creates a submodel object and returns to submodelObj. In the submodel this method assigns a value (NameValue) to the property Name assigns the model object (modelObj) to the property Parent. In model object, this method assigns the submodel object to the pro- Models.</pre>			
	modelObj = sbiomodel('cell') submodelObj = addmodel('nucleus')			



A model object must have a unique name at the level it is created. For example, if you create a model with the name cell, you cannot create another model object named cell. However, a model object can contain a submodel object named cell which can contain a submodel object named cell.

modelObj does not have access to submodelObj parameters. However, submodelObj does have access and can use modelObj parameters.

submodelObj = addmodel(...'PropertyName', PropertyValue...)
defines optional property values. The property name/property value
pairs can be in any format supported by the function set (for example,
name-value string pairs, structures, and name-value cell array pairs).

You can view additional model object properties with the function get. You can change additional model object properties with the function set. You can view the submodel objects of modelObj with the command get(modelObj, 'Models').

See Also sbiomodel, sbioupdate

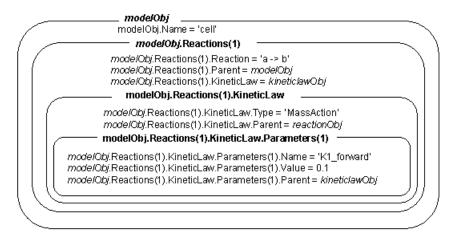
Create parameter object and add to model or kinetic law object		
parameterObj = addparameter( <i>Obj</i> , ' <i>NameValue</i> ') parameterObj = addparameter(Obj, ' <i>NameValue</i> ', <i>ValueValue</i> ) parameterObj = addparameter(' <i>PropertyName</i> ', <i>PropertyValue</i> )		
Obj	Model or kinetic law object. Enter a variable name for the object.	
NameValue	Property for a parameter object. Enter a unique character string. NameValue can be a cell array of parameter names. Since objects can use this property to reference a parameter, a parameter object must have a unique name at the level it is created. For example, a kinetic law object cannot contain two parameter objects named kappa. However, the model object that contains the kinetic law object can contain a parameter object named kappa along with the kinetic law object.	
For information on naming parameters, s Name.		
ValueValue	Property for a parameter object. Enter a number.	
<pre>parameterObj = addparameter(Obj, 'NameValue') creates a parameter object and returns the object (parameterObj). In the parameter object, this method assigns a value (NameValue) to the property Name, assigns a value 1 to the property Value, and assigns the model or kinetic law object to the property Parent. In the model or kinetic law object, (Obj), this method assigns the parameter object to the property Parameters. A parameter object defines an assignment that a model or a kinetic law can use. The scope of the parameter is defined by the parameter parent. If a parameter is defined with a kinetic law object, then only the</pre>		
	parameterObj = addpa parameterObj = addpa parameterObj = addpa <i>Obj</i> <i>NameValue</i> <i>ValueValue</i> parameterObj = addpa object and returns the this method assigns a a value 1 to the property this method assigns the A parameter object de law can use. The scop	

kinetic law object and objects within the kinetic law object can use the parameter. If a parameter object is defined with a model object as its parent, then all objects within the model (including all rules, events and kinetic laws) can use the parameter.

```
modelObj = sbiomodel('cell')
parameterObj = addparameter(modelObj, 'TF1', 0.01)

modelObj.Name = 'cell'
modelObj.Parameters(1)
modelObj.Parameters(1).Name = 'TF1'
modelObj.Parameters(1).Value = 0.01
modelObj.Parameters(1).Parent = modelObj
```

```
modelObj = sbiomodel('cell')
reactionObj = addreaction(modelObj, 'a -> b')
kineticlawObj = addkineticlaw (reactionObj, 'MassAction')
parameterObj = addparameter(kineticlawObj, 'K1_forward', 0.1)
```



parameterObj = addparameter(Obj, 'NameValue', ValueValue) creates a parameter object, assigns a value (NameValue) to the property Name, assigns the value (ValueValue) to the property Value, and assigns the model object or the kinetic law object to the property Parent. In the model or kinetic law object (Obj), this method assigns the parameter object to the property Parameters, and returns the parameter object to a variable (parameterObj).

parameterObj = addparameter(...'*PropertyName*', *PropertyValue*...) defines optional property values. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).

**Scope of a parameter** — A parameter can be *scoped* to either a model or a kinetic law.

- When a kinetic law searches for a parameter in its expression, it first looks in the parameter list of the kinetic law. If the parameter isn't found there, it moves to the model that the kinetic law object is in and looks in the model parameter list. If the parameter isn't found there, it moves to the model parent.
- When a rule searches for a parameter in its expression, it looks in the parameter list for the model. If the parameter isn't found there, it moves to the model parent. A rule cannot use a parameter that is scoped to a kinetic law. So for a parameter to be used in both a reaction rate equation and a rule, the parameter should be *scoped* to a model.

Additional parameter object properties can be viewed with the get command. Additional parameter object properties can be modified with the set command. The parameters of Obj can be viewed with get(*Obj*, 'Parameters').

A SimBiology parameter object can be copied to a SimBiology model or kinetic law object with copyobj. A SimBiology parameter object can be removed from a SimBiology model or kinetic law object with delete.

## addparameter (model, kineticlaw)

Method Summary	Methods for parameter objects		
Sommary	copyobj (any object)	Copy SimBiology object and its children	
	delete (any object)	Delete SimBiology object	
	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	
	rename (compartment, parameter, species)	Rename object and update expressions	
	set (any object)	Set object properties	
Property Summary	Properties for parameter objects		
	Annotation	Store link to URL or file	
	ConstantValue	Specify variable or constant parameter value	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	
	Parent	Indicate parent object	
	Tag	Specify label for SimBiology object	
	Туре	Display top-level SimBiology object type	
	UserData	Specify data to associate with object	
	Value	Assign value to parameter object	
	ValueUnits	Parameter value units	

Example	<b>1</b> Create a model object, and then add a reaction object.			
•	<pre>modelObj = sbiomodel ('my_model'); reactionObj = addreaction (modelObj, 'a + b -&gt; c + d');</pre>			
	<b>2</b> Define a kinetic law for the reaction object.			
	<pre>kineticlawObj = addkineticlaw(reactionObj, 'MassAction');</pre>			
	<b>3</b> Add a parameter and assign it to the kinetic law object (kineticlawObj); add another parameter and assign to the model object (modelObj).			
	% Add parameter to kinetic law object parameterObj1 = addparameter (kineticlawObj, 'K1');			
	get (kineticlawObj, 'Parameters')			
	MATLAB returns:			
	SimBiology Parameter Array			
	Index: Name: Value: ValueUnits: 1 K1 1			
	<pre>% Add parameter with value 0.9 to model object parameterObj1 = addparameter (modelObj, 'K2', 0.9); get (modelObj, 'Parameters') MATLAB returns: SimBiology Parameter Array</pre>			
	Index: Name: Value: ValueUnits: 1 K2 1			
See Also	addreaction			

Purpose	Add product species object to reaction object		
Syntax	<pre>speciesObj = addproduct(reactionObj, 'NameValue') speciesObj = addproduct(reactionObj, speciesObj) speciesObj = addproduct(reactionObj, 'NameValue',     Stoichcoefficient) speciesObj = addproduct(reactionObj, speciesObj,     Stoichcoefficient)</pre>		
Arguments	reactionObj	Reaction object. Enter a name for the reaction object.	
	NameValue	Property of a species object that names the object (not the reaction object). Enter a unique character string. For example, 'fructose 6-phosphate'. A species object can be referenced by other objects using this property. You can use the function sbioselect to find an object with a specific NameValue.	
	species0bj	Species object.	
	Stoichcoeffieient	Stoichiometric coefficients for products, length of array equal to length of NameValue, or length of speciesObj.	
Description	<pre>speciesObj = addproduct(reactionObj, 'NameValue') creates a species object and returns the species object (speciesObj). In the species object, this method assigns the value (NameValue) to the property Name. In the reaction object, this method assigns the species object to the property Products, modifies the reaction equation in the property Reaction to include the new species, and adds the stoichiometric coefficient 1 to the property Stoichiometry. When you define a reaction with a new species:</pre>		

- If no compartment objects exist in the model, the method creates a compartment object (called '*unnamed*') in the model and adds the newly created species to that compartment.
- If only one compartment object (compObj) exists in the model, the method creates a species object in that compartment.
- If there is more than one compartment object (compObj) in the model, you must qualify the species name with the compartment name.

For example, cell.glucose denotes that you want to put the species named glucose into a compartment named cell. Additionally, if the compartment named cell does not exist, the process of adding the reaction creates the compartment and names it cell.

Create and add a species object to a compartment object with the method addspecies.

speciesObj = addproduct(reactionObj, speciesObj), in the species object (speciesObj), assigns the parent object of the reactionObj to the species property Parent. In the reaction object (reactionObj), it assigns the species object to the property Products, modifies the reaction equation in the property Reaction to include the new species, and adds the stoichiometric coefficient 1 to the property Stoichiometry.

speciesObj = addproduct(reactionObj, 'NameValue', Stoichcoefficient), in addition to the description above, adds the stoichiometric coefficient (Stoichcoefficient) to the property Stoichiometry. If NameValue is a cell array of species names, then Stoichcoefficient must be a vector of doubles with the same length as NameValue.

speciesObj = addproduct(reactionObj, speciesObj, Stoichcoefficient), in addition to the description above, adds the stoichiometric coefficient (Stoichcoefficient) to the property Stoichiometry.

Species names are referenced by reaction objects, kinetic law objects, and model objects. If you change the Name of a species the reaction also

## addproduct (reaction)

	uses the new name. You must however configure all other applicable elements such as rules that use the species, and the kinetic law object.		
Examples	<b>1</b> Create a model object, and then add a reaction object.		
	<pre>modelObj = sbiomodel('my_model'); reactionObj = addreaction(modelObj, 'A + C -&gt; U');</pre>		
	<b>2</b> Modify the reaction of the reactionObj from A + C -> U to A + C -> U + 2 H.		
	<pre>speciesObj = addproduct(reactionObj, 'H', 2);</pre>		
See Also	addspecies, sbiospecies		

Purpose	Add species object as reactant to reaction object		
Syntax	<pre>speciesObj = addreactant(reactionObj, 'NameValue') addreactant(reactionObj, speciesObj, Stoichcoeffieient) addreactant(reactionObj, 'NameValue', Stoichcoeffieient)</pre>		
Arguments	reactionObjReaction object.NameValueName property of a species object. Enter a unique character string, for example, 'glucose'. A species object can be referenced by other objects using this property. You can use the function sbioselect to find an object with a specific Name property value.speciesObjSpecies object or cell array of species objects.StoichcoefficientStoichiometric coefficients for reactants, length of array equal to length of NameValue		
Description			

٠	If there is more than one compartment object (compObj) in the model,
	you must qualify the species name with the compartment name.

For example, cell.glucose denotes that you want to put the species named glucose into a compartment named cell. Additionally, if the compartment named cell does not exist, the process of adding the reaction creates the compartment and names it cell.

Create and add a species object to a compartment object with the method addspecies.

addreactant(reactionObj, speciesObj, Stoichcoeffieient), in the species object (speciesObj), assigns the parent object to the speciesObj property Parent. In the reaction object (reactionObj), it assigns the species object to the property Reactants, modifies the reaction equation in the property Reaction to include the new species, and adds the stoichiometric coefficient -1 to the property Stoichiometry. If speciesObj is a cell array of species objects, then Stoichcoeffieient must be a vector of doubles with the same length as speciesObj.

addreactant(reactionObj, 'NameValue', Stoichcoeffieient), in addition to the description above, adds the stoichiometric coefficient (Stoichcoeffieient) to the property Stoichiometry. If NameValue is a cell array of species names, then Coefficient must be a vector of doubles with the same length as NameValue.

Species names are referenced by reaction objects, kinetic law objects, and model objects. If you change the Name of a species the reaction also uses the new name. You must, however, configure all other applicable elements such as rules that use the species, and the kinetic law object.

See for more information on species names.

**Example** 1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'A -> U');
```

**2** Modify the reaction of the reactionObj from A -> U to be A + 3 C -> U.

speciesObj = addreactant(reactionObj, 'C', 3);

**See Also** addspecies, sbiospecies

Purpose	Create reaction object and add to model object		
Syntax	<pre>reactionObj = addreaction(modelObj,'ReactionValue') reactionObj = addreaction(modelObj, 'ReactantsValue',     'ProductsValue') reactionObj = addreaction(modelObj, 'ReactantsValue',     RStoichCoefficients, 'ProductsValue',     PStoichCoefficients) reactionObj = addreaction('PropertyName', PropertyValue)</pre>		

### Arguments

modelObj	SimBiology model object.
ReactionValue	Specify the reaction equation. Enter a character string. A hyphen preceded by a space and followed by a right angle bracket (->) indicates reactants going forward to products. A hyphen with left and right angle brackets (<->) indicates a reversible reaction. Coefficients before reactant or product names must be followed by a space.
	Examples are 'A -> B', 'A + B -> C', '2 A + B -> 2 C', and 'A <-> B'. Enter reactions with spaces between the species.
	If there are multiple compartments, or to specify the compartment name, use <i>compartmentName.speciesName</i> .
	Examples are 'cytoplasm.A -> cytoplasm.B', 'cytoplasm.A -> nucleus.A', and 'cytoplasm.A + cytoplasm.B -> nucleus.AB'.

	ReactantsValue	A string defining the species name, a cell array of strings, a species object, or an array of species objects. If using name strings, qualify with compartment names if there are multiple compartments.
	ProductsValue	A string defining the species name, a cell array of strings, a species object, or an array of species objects. If using name strings, qualify with compartment names if there are multiple compartments.
	RStoichCoefficients	Stoichiometric coefficients for reactants, length of array equal to length of <i>ReactantsValue</i> .
	PStoichCoefficients	Stoichiometric coefficients for products, length of array equal to length of <i>ProductsValue</i> .
Description	<pre>reactionObj = addreaction(modelObj, 'ReactionValue') creates a reaction object, assigns a value (ReactionValue) to the property Reaction, assigns reactant species object(s) to the property Reactants, assigns the product species object(s) to the property Products, and assigns the model object to the property Parent. In the Model object (modelObj), this method assigns the reaction object to the property</pre>	

<pre>reactionObj = addreaction(modelObj,</pre>	'a ->	b')
modelObj modelObj.Name = 'cell' modelObj.Reactions(1)		
mode/Obj.Reactions(1).Reaction = 'a -> b' mode/Obj.Parameters(1).Parent = mode/Obj		

Reactions, and returns the reaction object (reactionObj).

When you define a reaction with a new species:

- If no compartment objects exist in the model, the method creates a compartment object (called '*unnamed*') in the model and adds the newly created species to that compartment.
- If only one compartment object (compObj) exists in the model, the method creates a species object in that compartment.
- If there is more than one compartment object (compObj) in the model, you must qualify the species name with the compartment name.

For example, cell.glucose denotes that you want to put the species named glucose into a compartment named cell. Additionally, if the compartment named cell does not exist, the process of adding the reaction creates the compartment and names it cell.

You can manually add a species to a compartment object with the method addspecies.

You can add species to a reaction object using the methods addreactant or addproduct. You can remove species from a reaction object with the methods rmreactant or rmproduct. The property Reaction is modified by adding or removing species from the reaction equation.

You can copy a SimBiology reaction object to a model object with the function copyobj. You can remove the SimBiology reaction object from a SimBiology model object with the function delete.

You can view additional reaction object properties with the get command. For example, the reaction equation of reactionObj can be viewed with the command get(*reactionObj*, 'Reaction'). You can modify additional reaction object properties with the command set.

reactionObj = addreaction(modelObj, 'ReactantsValue', 'ProductsValue') creates a reaction object, assigns a value to the property Reaction using the reactant (ReactantsValue) and product (ProductsValue) names, assigns the species objects to the properties Reactants and Products, and assigns the model object to the property Parent. In the model object (modelObj), this method assigns the reaction object to the property Reactions, and returns the reaction object (reactionObj). The stoichiometric values are assumed to be 1.

	<pre>reactionObj = addreaction(modelObj, 'ReactantsValue', RStoichCoefficients, 'ProductsValue', PStoichCoefficients) adds stoichiometric coefficients (RStoichCoefficients) for reactant species, and stoichiometric coefficients (PStoichCoefficients) for product species to the property Stoichiometry. The length of Reactants and RCoefficients must be equal, and the length of Products and PCoefficients must be equal. reactionObj = addreaction('PropertyName', PropertyValue) defines optional properties. The property name/property value pairs can be in any format supported by the function set (for example, name-value string pairs, structures, and name-value cell array pairs).</pre>		
Method Methods for reaction objects			
Summary	addkineticlaw (reaction)	Create kinetic law object and add to reaction object	
	addproduct (reaction)	Add product species object to reaction object	
	addreactant (reaction)	Add species object as reactant to reaction object	
	copyobj (any object)	Copy SimBiology object and its children	
	delete (any object)	Delete SimBiology object	
	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	
	rmproduct (reaction)	Remove species object from reaction object products	
	rmreactant (reaction)	Remove species object from reaction object reactants	
	set (any object)	Set object properties	

## addreaction (model)

Property Summary	Properties for reaction objects	
John any	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	KineticLaw	Show kinetic law used for ReactionRate
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Products	Array of reaction products
	Reactants	Array of reaction reactants
	Reaction	Reaction object reaction
	ReactionRate	Reaction rate equation in reaction object
	Reversible	Specify whether reaction is reversible or irreversible
	Stoichiometry	Species coefficients in reaction
	Tag	Specify label for SimBiology object
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object

## **Examples** Create a model, add a reaction object, and assign the expression for the reaction rate equation.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

2 Create a kinetic law object for the reaction object, of the type 'Henri-Michaelis-Menten'.

kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');

reactionObj KineticLaw property is configured to kineticlawObj.

3 The 'Henri-Michaelis-Menten' kinetic law has two parameter variables (Vm and Km) and one species variable (S) that should to be set. To set these variables, first create the parameter variables as parameter objects (parameterObj1, parameterObj2) with names Vm\_d, and Km\_d, and assign the objects Parent property value to the kineticlawObj.

```
parameterObj1 = addparameter(kineticlawObj, 'Vm_d');
parameterObj2 = addparameter(kineticlawObj, 'Km d');
```

**4** Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Vm_d' 'Km_d'});
set(kineticlawObj,'SpeciesVariableNames', {'a'});
```

**5** Verify that the reaction rate is expressed correctly in the reaction object ReactionRate property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =
```

```
Vm_d*a/(Km_d+a)
```

**See Also** addkineticlaw, addproduct, addreactant, rmproduct, rmreactant

## addrule (model)

Purpose	Create rule object and add to model object	
Syntax	<pre>ruleObj = addrule(modelObj, 'RuleValue') ruleObj = addrule(modelObj, 'RuleValue', 'RuleTypeValue') ruleObj = addrule(, 'PropertyName', PropertyValue,)</pre>	
Arguments	modelObj	Model object to which to add the rule.
	RuleValue	Enter a character string within quotation marks. For example, enter the algebraic rule 'Va*Ea + Vi*Ei - K2'.
	RuleTypeValue	Enter 'algebraic', 'initialassignment', 'repeatedAssignment', or 'rate'. See RuleType for more information.

## **Description** A rule is a mathematical expression that changes the amount of a species or the value of a parameter. It also defines how species and parameters interact with one another.

ruleObj = addrule(modelObj, 'RuleValue') creates a rule object and returns the rule object (ruleObj). In the rule object, this method assigns a value ('RuleValue') to the property Rule, assigns the value 'algebraic' to the property RuleType, and assigns the model object (modelObj) to the property Parent. In the model object (modelObj), this method assigns the rule object to the property Rules.

ruleObj = addrule(modelObj, 'RuleValue', 'RuleTypeValue') in addition to the assignments above, assigns a value (RuleTypeValue) to the property RuleType. For more information on the different types of rules, see RuleType.

ruleObj = addrule(..., 'PropertyName', PropertyValue,...) defines
optional properties. The property name/property value pairs can be in
any format supported by the function set (for example, name-value
string pairs, structures, and name-value cell array pairs).

	properties with the function s	es with the function get, and modify rule set. Copy a rule object to a model with te a rule object from a model with the
Method	Methods for rule objects	
Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	set (any object)	Set object properties
Property Summary	Properties for rule objects	
Johnnary	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Rule	Specify species and parameter interactions
	RuleType	Specify type of rule for rule object
	Tag	Specify label for SimBiology object

	Type UserData	Display top-level SimBiology object type Specify data to associate with object
Examples	modelObj = sbio ruleObj = addru 2 Get a list of properti	et, and then add a rule object. omodel('cell'); wle(modelObj, '0.1*B-A')
	MATLAB displays a list of rule properties. Active: 1 Annotation: '' Name: '' Notes: '' Parent: [1x1 SimBiology.Model] Rule: '0.1*B-A' RuleType: 'algebraic' Tag: '' Type: 'rule' UserData: []	

Add a rule with the RuleType property set to rate.

**1** Create model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a -> b');
```

**2** Add a rule which defines that the quantity of a species c. In the rule expression, k is the rate constant for  $a \rightarrow b$ .

```
ruleObj = addrule(modelObj, 'c = k*(a+b)')
```

**3** Change the RuleType from default ('algebraic') to 'rate', and verify using the get command.

```
set(ruleObj, 'RuleType', 'rate');
get(ruleObj)
```

MATLAB returns all the properties for the rule object.

```
Active: 1
Annotation: ''
Name: ''
Parent: [1x1 SimBiology.Model]
Rule: 'c = k*(a+b)'
RuleType: 'rate'
Tag: ''
Type: 'rule'
UserData: []
```

See Also copyobj, delete, sbiomodel

Purpose	Create species object and add to compartment object	
Syntax	<pre>speciesObj = addspecies(compObj, 'NameValue') speciesObj = addspecies(compObj, 'NameValue',     InitialAmountValue) speciesObj = addspecies('PropertyName', PropertyValue)</pre>	
Arguments	compObj	Compartment object.
	NameValue	Name for a species object. Enter a character string unique within <i>compObj</i> . Species objects are identified by name within Event, ReactionRate, and Rule property strings. For information on naming species, see Name.
		You can use the function sbioselect to find an object with a specific Name property value.
	InitialAmountValue	Initial amount value for the species object. Enter double. Positive real number, default = 0.
	PropertyName	Enter the name of a valid property. Valid property names are listed in "Property Summary" on page 4-52.
	PropertyValue	Enter the value for the property specified in <i>PropertyName</i> . Valid property values are listed on each property reference page.
Description		es(compObj, 'NameValue') creates a species species object (speciesObj). In the species

object and returns the species (composition), inductive (strates a species object and returns the species object (speciesObj). In the species object, this method assigns a value (NameValue) to the property Name, and assigns the compartment object (compObj) to the property Parent. In the compartment object, this method assigns the species object to the property Species.

```
speciesObj = addspecies(compObj, 'NameValue',
InitialAmountValue), in addition to the above, assigns an initial
amount (InitialAmountValue) for the species.
```

You can also add a species to a reaction using the methods addreactant and addproduct.

A species object must have a unique name at the level at which it is created. For example, a compartment object cannot contain two species objects named H20. However, another compartment can have a species named H20.

View properties for a species object with the get command, and modify properties for a species object with the set command. You can view a summary table of species objects in a compartment (compObj) with get(compObj, 'Species') or the properties of the first species with get(compObj.Species(1)).

speciesObj = addspecies(...'PropertyName', PropertyValue...)
defines optional properties. The property name/property value pairs
can be in any format supported by the function set (for example,
name-value string pairs, structures, and name-value cell array pairs).
The property summary on this page shows the list of properties.

If there is more than one compartment object (compObj) in the model, you must qualify the species name with the compartment name. For example, cell.glucose denotes that you want to put the species named glucose into a compartment named cell. Additionally, if the compartment named cell does not exist, the process of adding the reaction creates the compartment and names it cell.

If you change the name of a species you must configure all applicable elements, such as events and rules that use the species, any user-specified ReactionRate, or the kinetic law object property SpeciesVariableNames. Use the method setspecies to configure SpeciesVariableNames.

To update species names in the SimBiology graphical user interface, access each appropriate pane through the **Project Explorer**. You can also use the **Find** feature to locate the names that you want to update.

	The <b>Output</b> pane opens with the results of <b>Find</b> . Double-click a result row to go to the location of the model component.		
	Species names are automatically updated for reactions that use MassAction kinetic law.		
Method Summary	Methods for species objects		
Sommary	copyobj (any object)	Copy SimBiology object and its children	
	delete (any object)	Delete SimBiology object	
	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	
	rename (compartment, parameter, species)	Rename object and update expressions	
	set (any object)	Set object properties	
Property Summary	Properties for species objects		
Joinna y	Annotation	Store link to URL or file	
	BoundaryCondition	Indicate species boundary condition	
	ConstantAmount	Specify variable or constant species amount	
	InitialAmount	Species initial amount	
	InitialAmountUnits	Species initial amount units	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	
	Parent	Indicate parent object	

	Тад	Specify label for SimBiology object	
	Туре	Display top-level SimBiology object type	
	UserData	Specify data to associate with object	
Examples	Add two species to a mode enzyme catalyzing the rea	l, where one is a reactant and the other is the ction.	
	<ol> <li>Create a model object n object.</li> </ol>	amed my_model and add a compartment	
	modelObj = sbiomo compObj = addcomp	del ('my_model'); artment(modelObj, 'comp1');	
		two species objects named glucose_6_phosphate and ose_6_phosphate_dehydrogenase.	
		species (compObj, 'glucose_6_phosphate'); species (compObj, 'glucose_6_phosphate_dehydrogenase');	
	<b>3</b> Set the initial amount of	f glucose_6_phosphate to 100 and verify.	
	set (speciesObj1, get (speciesObj1,	'InitialAmount',100); 'InitialAmount')	
	MATLAB returns:		
	ans =		
	100		
	<b>4</b> Use get to note that mo	delObj contains the species object array.	
	get(compObj, 'Spe	cies')	

MATLAB returns:

SimBiology Species Array

Index: Name:

InitialAmount: InitialAmountUnits:

- 1 glucose\_6\_phosphate
  - 100
- 2 glucose\_6\_phosphate\_dehydrogenase 0

**5** Retrieve information about the first species in the array.

See Also addcompartment, addproduct, addreactant, addreaction, get, set

Purpose	Add variant to model		
Syntax	variantObj = addvariant(modelObj, 'NameValue') variantObj2 = addvariant(modelObj, variantObj)		
Arguments	mode10bj	Specify the model object to which you want add a variant.	
	variant0bj	Variant object to create and add to the model object.	
	NameValue	Name of the variant object. <i>NameValue</i> is assigned to the Name property of the variant object.	
Description	<pre>variantObj = addvariant(modelObj, 'NameValue') creates a SimBiology variant object (variantObj) with the name NameValue and adds the variant object to the SimBiology model object modelObj. The variant object Parent property is assigned the value of modelObj.</pre>		
	A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see Variant object.		
	<pre>variantObj2 = addvariant(modelObj, variantObj) adds a SimBiology variant object (variantObj) to the SimBiology model object and returns another variant object variantObj2. The variant object variantObj2 Parent property is assigned the value of modelObj.</pre>		
	View properties for a variant object with the get command, and modify properties for a variant object with the set command.		
	<b>Note</b> Remember to use the addcontent method instead of using the set method on the Content property, because the set method replaces the data in the Content property, whereas addcontent appends the data.		

To view the variants stored on a model object, use the getvariant method. To copy a variant object to another model, use copyobj. To remove a variant object from a SimBiology model, use the delete method.

Examples	1 Create a model containing one species.	
	<pre>modelObj = sbiomodel('mymodel'); compObj = addcompartment(modelObj, 'comp1'); speciesObj = addspecies(compObj, 'A');</pre>	
	<b>2</b> Add a variant object that varies the InitialAmount property of a species named A.	
	variantObj = addvariant(modelObj, 'v1'); addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});	
See Also	addcontent, commit, copyobj, delete, getvariant	

#### **Purpose** Solver settings information for model simulation

# **Description** The SimBiology configset object, also known as the configuration set object, contains the options that the solver uses during simulation of the model object. The configuration set object contains the following options for you to choose:

- Type of solver
- Stop time for the simulation
- Solver error tolerances, and for ode solvers the maximum time step the solver should take
- Whether to perform sensitivity analysis during simulation
- Whether to perform dimensional analysis and unit conversion during simulation
- Species and parameter input factors for sensitivity analysis

A SimBiology model can contain multiple configsets with one being active at any given time. The active configset contains the settings that are used during the simulation. Use the method setactiveconfigset to define the active configset. Use the method getconfigset to return a list of configsets contained by a model. Use the method addconfigset to add a new configset to a model.

See "Property Summary" on page 4-58 for links to configset object property reference pages.

Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the SimBiology desktop.

Constructor Summary

addconfigset (model)

Create configuration set object and add to model object

## Configset object

Method Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	set (any object)	Set object properties
Property Summary	Active	Indicate object in use during simulation
	CompileOptions	Dimensional analysis and unit conversion options
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	RuntimeOptions	Options for logged species
	SensitivityAnalysisOptions	Specify sensitivity analysis options
	SolverOptions	Specify model solver options
	SolverType	Select solver type for simulation
	StopTime	Set stop time for simulation
	StopTimeType	Specify type of stop time for simulation
	TimeUnits	Show stop time units for simulation
	Туре	Display top-level SimBiology object type

See Also AbstractKineticLaw object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Rule object, Species object

## commit (variant)

Purpose	Commit variant contents to model		
Syntax	commit(variantObj,	<pre>commit(variantObj, modelObj)</pre>	
Arguments	modelObj variantObj	Specify the model object to which you want to commit a variant. Variant object to commit to the model object.	
Description	<pre>commit(variantObj, modelObj) commits the Contents property of a SimBiology variant object (variantObj) to the model object modelObj. The property values stored in the variant object replace the values stored in the model.</pre>		
	A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see Variant object.		
	duplicate entries ov	et on the model object in order of occurrence, with erwriting. If the commit method finds an incorrectly rror occurs and the remaining properties defined in rty are not set.	
Examples	modelObj = s compObj = ad	ontaining one species. biomodel('mymodel'); dcompartment(modelObj, 'comp1'); addspecies(compObj, 'A', 10);	
	species named A. variantObj =	<pre>iect that varies the InitialAmount property of a     addvariant(modelObj, 'v1'); ariantObj, {'species', 'A', 'InitialAmount', 5});</pre>	
	<b>3</b> Commit the conte	ents of the variant (variantObj).	

commit (variantObj, modelObj);

See Also addvariant, Variant object

## Compartment object

Purpose	Options for compartments			
Description	The SimBiology compartment object represents a container for species in a model. Compartment size can vary or remain constant during a simulation. All models must have at least one compartment and all species in a model must be assigned to a compartment. Compartment names must be unique within a model.			
Compartments allow you to define the size (Capacity) of physically isolated regions that may affect simulation, and associate pools of species within those regions. You can specify or change Capacity u rules, events, and variants, similar to species amounts or parameter values. The model object stores compartments as a flat list. Each compartment stores information on its own organization; in other words a compartment has information on which compartment it lives within (Owner) and who it contains (Compartments). The flat list of compartments in the model object lets you vary the w compartments are organized in your model without invalidating an expressions.				
			To add species that participate in reactions, add the reaction to th model using the addreaction method. When you define a reaction a new species:	
			• If no compartment objects exist in the model, the addreaction method creates a compartment object (called ' <i>unnamed</i> ') in the model and adds the newly created species to that compartment.	
<ul> <li>If only one compartment object exists in the model, the meth creates a species object in that compartment.</li> <li>If there is more than one compartment object in the model, yo qualify the species name with the compartment name.</li> </ul>				
			For example, cell.glucose denotes that you want to put the species named glucose into a compartment named cell. Additionally, if the	

compartment named cell does not exist, the process of adding the reaction creates the compartment and names it cell.

Alternatively, create and add a species object to a compartment object, using the addspecies method at the command line.

The SimBiology desktop adds a default compartment (*unnamed*) for you and you can add a species in the **Species** pane. In the **Project Explorer**, expand **Compartment** and double-click **Species** to open the **Species** pane.

You can specify reactions that cross compartments using the syntax compartment1Name.species1Name -> compartment2Name.species2Name. If you add a reaction that contains species from different compartments, and the reaction rate dimensions are concentration/time, all reactants should be from the same compartment.

In addition, if the reaction is reversible then there are two cases:

- If the kinetic law is MassAction, and the reaction rate reaction rate dimensions are concentration/time, then the products must be from the same compartment.
- If the kinetic law is not MassAction, then both reactants and products must be in the same compartment.

See "Property Summary" on page 4-64 for links to compartment property reference pages. Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

#### Constructor a Summary c

addcompartment (model, compartment)

Create compartment object

## Compartment object

Method Summary	Methods for compartment objects	
	addcompartment (model, compartment)	Create compartment object
	addspecies (compartment)	Create species object and add to compartment object
	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	rename (compartment, parameter, species)	Rename object and update expressions
	reorder (model, compartment)	Reorder component lists
	set (any object)	Set object properties
Property Summary	Properties for compartment objects	3
	Annotation	Store link to URL or file
	Capacity	Compartment capacity
	CapacityUnits	Compartment capacity units
	Compartments	Array of compartments in model or compartment
	ConstantCapacity	Specify variable or constant compartment capacity
	Name	Specify name of object
	Notes	HTML text describing SimBiology object

Owner	Owning compartment
Parent	Indicate parent object
Species	Array of species in compartment object
Tag	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

See Also AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Rule object

### copyobj (any object)

Purpose	Copy SimBiology object and its children		
Syntax	copiedObj = copyobj(Obj, parentObj) copiedObj = copyobj(modelObj)		

#### Arguments

Abstract kinetic law, compartment, configuration set, event, kinetic law, model, parameter, reaction, rule, species, or variant object.

parent0bj

model0bj

0bj

If copiedObj is	parentObj must be
configuration set, event, reaction, rule, or variant object	model object
compartment object	compartment or model object
species object	compartment object
parameter object	model or kinetic law object
kinetic law object	reaction object
model object or abstract kinetic law object	sbioroot

copiedObj Output returned by the copyobj method with the parent set as specified in input argument (parentObj).

**Description** copiedObj = copyobj(Obj, parentObj) makes a copy of a SimBiology object (Obj) and returns a pointer to the copy (copiedObj). In the copied object (copiedObj), this method assigns a value (parentObj) to the property Parent.

	<pre>copiedObj = copyobj(modelObj) makes a copy of a model object (modelObj) and returns the copy (copiedObj). In the copied model object (copiedObj), this method assigns the root object to the property Parent.</pre>		
Examples	Create a reaction object separate from a model object, and then add it to a model.		
	Create a model object and add a reaction object.		
	<pre>modelObj1 = sbiomodel('cell'); reactionObj = addreaction(modelObj1, 'a -&gt; b');</pre>		
	<b>2</b> Create a copy of the reaction object and assign it to another model object.		
	<pre>modelObj2 = sbiomodel('cell2'); reactionObjCopy = copyobj(reactionObj, modelObj2); modelObj2.Reactions</pre>		
SimBiology Reaction Array			
	Index: Reaction: 1 a -> b		
<b>~</b> • •			

See Also sbiomodel, sbioroot

## delete (any object)

Purpose	Delete SimBiology object		
Syntax	<pre>delete(Obj)</pre>		
Arguments	Obj	SimBiology object: abstract kinetic law, configuration set, kinetic law, model, parameter, reaction, rule, or species.	
Description	<ul> <li>delete(Obj) removes an object (Obj) from its parent.</li> <li>If Obj is a species object that is being used by a reaction object, this method returns an error and the species object is not deleted. You need to delete the reaction or remove the species from the reaction</li> </ul>		
	<ul> <li>before you can delete the species object.</li> <li>If <i>Obj</i> is a parameter object being used by a kinetic law object, there is no warning when the object is deleted. However, when you try to simulate your model, a error occurs because the parameter cannot be found.</li> </ul>		
	• If <i>Obj</i> is a reaction object, this method deletes the object, but the species objects that were being used by the reaction object are not deleted.		
	• If <i>Obj</i> is an abstract kinetic law object and there is a kinetic law object referencing it, this method returns an error.		
	• If <i>Obj</i> is a SimBiology configuration set object, and it is the active configuration set object, this method, after deleting the object, makes the default configuration set object active. Note that you cannot delete the default configuration set.		
	• You cannot delete the SimBiology root.		
	You can also delete all model objects from the root with one call to the sbioreset function.		

#### **Examples** Example 1

Delete a reaction from a model. Notice the species objects are not deleted with the reaction object.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'a -> b');
delete(reactionObj)
```

#### Example 2

Delete a single model from the root object.

```
modelObj1 = sbiomodel('cell');
modelObj2 = sbiomodel('virus');
delete(ModelObj2)
```

See Also sbiomodel, sbioreset, sbioroot

## display (any object)

Purpose	Display summary of SimBiology object	
Syntax	display(Obj)	
Arguments	Obj	SimBiology object: abstract kinetic law, configuration set, compartment, event, kinetic law, model, parameter, reaction, rule, species, or unit.
Description	Display the SimBiology object array. display(Obj) is called for the SimBiology object, Obj when the semicolon is not used to terminate a statement. The display of Obj gives a brief summary of the Obj configuration. You can view a complete list of Obj properties with the command get. You can modify all Obj properties that can be changed, with the command set.	
Examples	<pre>modelObj = sbiomodel('cell') reactionObj = addreaction(modelObj, 'A + B -&gt; C')</pre>	

#### **Purpose**Store event information

# **Description** Events are used to describe sudden changes in model behavior. An event lets you specify discrete transitions in model component values that occur when a user-specified condition become true. You can specify that the event occurs at a particular time, or specify a time-independent condition.

For details on how events are handled during a simulation, see "Changing Model Component Values Using Events" in the SimBiology User's Guide documentation.

See "Property Summary" on page 4-72 for links to event property reference pages.

Properties define the characteristics of an object. For example, an event object includes properties that allow you to specify the conditions to trigger an event (Trigger), and what to do after the event is triggered (EventFcn). Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the SimBiology desktop.

Constructor Summary	addevent (model)	Add event object to model object
Method Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	set (any object)	Set object properties

### **Event object**

Property Summary	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	EventFcns	Event expression
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Tag	Specify label for SimBiology object
	Trigger	Event trigger
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object
See Also	AbstractKingticlaw object Co	nfigset object Kineticlaw

See Also AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Rule object, Species object

Purpose	Get object properties	
Syntax	<pre>PropertyValue = get(Obj, 'PropertyName') objProperties = get(Obj)</pre>	
Arguments	PropertyValue Value defined for 'PropertyName'	
	Obj	Abstract kinetic law, compartment, configuration set, event, kinetic law, model, parameter, reaction, rule, species, or variant object.
	'PropertyName'	Name of the property to get. For properties that you can get for each object, see AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Parameter object, Reaction object, Rule object, Species object, Variant object
	objProperties	Struct containing properties and values for the object, <i>Obj</i> .

Description	<pre>PropertyValue = get(Obj, 'PropertyName') gets the value 'PropertyValue' of the object, Obj's PropertyName property.</pre>		
	<i>objProperties</i> = get( <i>Obj</i> ) gets the properties for the object, <i>Obj</i> , and returns it to <i>objProperties</i> .		
Examples	<pre>I Create a model object. modelObj = sbiomodel ('my_model');</pre>		
	2 Add parameter object.		

```
parameterObj = addparameter (modelObj, 'kf');
3 Set the ConstantValue property of the parameter object to false
and verify.
MATLAB returns 1 for true and 0 for false.
set (parameterObj, 'ConstantValue', false);
get(parameterObj, 'ConstantValue')
MATLAB returns
ans =
0
```

See Also getadjacencymatrix, getconfigset, getdata, getparameters, getsensmatrix, getspecies, getstoichmatrix, set

Purpose	Get adjacency matrix from model object	
Syntax	<pre>M = getadjacencymatrix(modelObj) M = getadjacencymatrix(modelObj,'flat') [M, Headings] = getadjacencymatrix(modelObj) [M, Headings, Mask] = getadjacencymatrix(modelObj)</pre>	
Arguments	M Adjacency matrix for modelObj.	
	modelObj	Specify the model object.
	'flat'	Return adjacency matrix for only specified <i>modelObj</i> , not for objects contained in the <i>modelObj</i> .
	Headings	Return row and column headings. If species are in multiple compartments, species names are qualified with the compartment name in the form compartmentName.speciesName. For example, nucleus.DNA, cytoplasm.mRNA.
	MaskReturn 1 for the species object and 0 for the reaction object to Mask.	
Description	getadjacencymatrix returns the adjacency matrix for a model object.	
	M = getadjacencymatrix(modelObj) returns an adjacency matrix for the model object (modelOBJ) to $M$ .	
	An adjacency matrix is defined by listing all species contained by <i>modelObj</i> and all reactions contained by <i>modelObj</i> column-wise and row-wise in a matrix. The reactants of the reactions are represented in the matrix with a 1 at the location of [row of species, column of reaction]. The products of the reactions are represented in the matrix with a 1 at the location of [row of reaction, column of species]. All other locations in the matrix are 0.	

	<pre>M = getadjacencymatrix(modelObj,'flat') returns the adjacency matrix to M and defines the adjacency matrix for only modelObj. M is the adjacency matrix for the reactions and species contained by modelObj.</pre>		
	[ <i>M</i> , <i>Headings</i> ] = getadjacencymatrix( <i>modelObj</i> ) returns the adjacency matrix to M and the row and column headings to <i>Headings</i> . <i>Headings</i> is defined by listing all Name property values of species contained by <i>modelObj</i> and all Name property values of reactions contained by <i>modelObj</i> .		
	[ <i>M</i> , <i>Headings</i> , <i>Mask</i> ] = getadjacencymatrix( <i>modelObj</i> ) returns an array of 1s and 0s to <i>Mask</i> , where a 1 represents a species object and a 0 represents a reaction object.		
Examples	1 Read in a model using sbmlimport.		
	<pre>modelObj = sbmlimport('lotka.xml');</pre>		
	<b>2</b> Get the adjacency matrix for the modelObj.		
	<pre>[M, Headings] = getadjacencymatrix(modelObj)</pre>		
See Also	getstoichmatrix		

Purpose	Get configuration set object from model object	
Syntax	configsetObj = g	etconfigset(modelObj, 'NameValue') etconfigset(modelObj) etconfigset(modelObj,'active')
Arguments	modelObj NameValue	Model object. Enter a variable name for a model object. Name of the configset object.
	configsetObj	Object holding the simulation-specific information.
Description	<pre>configsetObj = getconfigset(modelObj, 'NameValue') returns the configuration set attached to modelObj that is named NameValue, to configsetObj. configsetObj = getconfigset(modelObj) returns a vector of all attached configuration sets, to configsetObj.</pre>	
	<i>configset0bj</i> = g configuration set.	<pre>etconfigset(modelObj,'active') retrieves the active</pre>
	SimBiology model active at any give	et object stores simulation-specific information. A l can contain multiple configsets with one being n time. The active configuration set contains the used during the simulation.
	<i>mode10bj</i> always configured to 'det	econfigset function to define the active configset. contains at least one configset object with the name fault'. Additional configset objects can be added the method addconfigset.
Examples	<b>1</b> Retrieve the de	fault configset object from the modelObj.
	-	= sbiomodel('cell'); bj = getconfigset(modelObj)

Configuration Settings - default (active) SolverType: ode15s StopTime: 10.000000 SolverOptions: AbsoluteTolerance: 1.000000e-006 RelativeTolerance: 1.000000e-003 RuntimeOptions: StatesToLog: all CompileOptions: UnitConversion: true DimensionalAnalysis: true **2** Configure the SolverType to ssa. set(configsetObj, 'SolverType', 'ssa') get(configsetObj) Active: 1 CompileOptions: [1x1 SimBiology.CompileOptions] Name: 'default' Notes: '' RuntimeOptions: [1x1 SimBiology.RuntimeOptions] SolverOptions: [1x1 SimBiology.SSASolverOptions] SolverType: 'ssa' StopTime: 10 StopTimeType: 'simulationTime' TimeUnits: 'second' Type: 'configset' addconfigset, removeconfigset, setactiveconfigset

See Also

Purpose	Get data from	Get data from SimData object array	
Syntax		[t, x, names] = getdata(simDataObj) [Out] = getdata(simDataObj, 'FormatValue')	
Arguments	Output Arg	Output Arguments	
	t	An n-by-1 vector of time points.	
	X	An n-by-m data array. <i>t</i> and <i>names</i> label the rows and columns of <i>x</i> respectively.	
	names	An m-by-1 cell array of names.	
	Metadata	When used with the 'nummetadata' input argument, <i>Metadata</i> contains a cell array of metadata structures. The elements of <i>Metadata</i> label the columns of <i>x</i> .	
	Out	Data returned in the format specified in 'FormatValue', shown in "Input Arguments" on page 4-79. Depending on the specified 'FormatValue', Out contains one of the following:	
		• Structure array	
		• SimData object	
		• Time series object	
		<ul> <li>Combined time series object from an array of SimData objects</li> </ul>	

#### **Input Arguments**

simDataObj	SimData object. Enter a variable name for a SimData object.
FormatValue	Choose a format from the following table.

FormatValue	Description
'num'	Specifies the format that lets you return data in numeric arrays. This is the default when getdata is called with multiple output arguments.
'nummetadata'	Specifies the format that lets you return a cell array of metadata structures in $metadata$ instead of names. The elements of $metadata$ label the columns of $x$ .
'numqualnames'	Specifies the format that lets you return qualified names in <i>names</i> to resolve ambiguities.
'struct'	Specifies the format that lets you return a structure array holding both data and metadata. This is the default when you use a single output argument.
'simdata'	Specifies the format that lets you return data in a new SimData object. This format is more useful for SimData methods other than getdata.

FormatValue	Description
'ts'	Specifies the format that lets you return data in time series objects, creating an individual time series for each state or column and SimData object in simDataObj.
'tslumped'	Specifies the format that lets you return data in time series objects, combining data from each SimData object into a single time series.

**Description** [t, x, names] = getdata(simDataObj) gets simulation time and state data from the SimData object simDataObj. When simDataObj contains more than one element, the outputs t, x, names are cell arrays in which each cell contains data for the corresponding element of simDataObj.

[Out] = getdata(simDataObj, 'FormatValue') returns the data in the specified format. Valid formats are listed in "Input Arguments" on page 4-79.

#### **Examples** Simulating and Retrieving Data

1 The project file, radiodecay.sbproj, contains a model stored in a variable called m1. Load m1 into the MATLAB workspace and simulate the model.

```
sbioloadproject('radiodecay');
simDataObj = sbiosimulate(m1);
```

2 Get all the simulation data from the SimData object.

[t x names] = getdata(simDataObj);

#### **Retrieving Data for Ensemble Runs**

1 The project file, radiodecay.sbproj, contains a model stored in a variable called m1. Load m1 into the MATLAB workspace.

```
sbioloadproject('radiodecay');
```

**2** Change the solver to use during the simulation and perform an ensemble run.

```
csObj = getconfigset(m1);
set(csObj, 'SolverType', 'ssa');
simDataObj = sbioensemblerun(m1, 10);
```

**3** Get all the simulation data from the SimData object.

```
tsObjs = getdata(simDataObj(1:5), 'ts');
```

See Also display, get, resample, selectselectbyname, setactiveconfigset MATLAB function struct

Purpose	Get specific parameters in kinetic law object	
Syntax	<pre>parameterObj = getparameters(kineticlawObj) parameterObj = getparameters(kineticlawObj,</pre>	
Arguments	kineticlawObj	Retrieve parameters used by the kinetic law object.
	ParameterVariablesValue	Retrieve parameters used by the kinetic law object corresponding to the specified parameter in the ParameterVariables property of the kinetic law object.
Description	<pre>parameterObj = getparameters(kineticlawObj) returns the parameters used by the kinetic law object kineticlawObj to parameterObj.</pre>	
	<pre>parameterObj = getparameters(kineticlawObj, 'ParameterVariablesValue') returns the parameter in the ParameterVariableNames property that corresponds to the parameter specified in the ParameterVariables property of kineticlawObj, to parameterObj. ParameterVariablesValue is the name of the parameter as it appears in the ParameterVariables property of kineticlawObj. ParameterVariablesValue can be a cell array of strings.</pre>	
	If you change the name of a para applicable elements such as rules user-specified ReactionRate, or t ParameterVariableNames. Use th ParameterVariableNames.	s that use the parameter, any
Examples	Create a model, add a reaction, and for the reaction rate equation.	${ m d} { m assign} { m the} { m ParameterVariableNames}$

**1** Create the model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

2 Create a kinetic law object for the reaction object, of the type 'Henri-Michaelis-Menten'.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

**3** Add two parameter objects.

```
parameterObj1 = addparameter(kineticlawObj,'Va');
parameterObj2 = addparameter(kineticlawObj,'Ka');
```

**4** The 'Henri-Michaelis-Menten' kinetic law has two parameter variables (Vm and Km) that should to be set. To set these variables:

setparameter(kineticlawObj,'Vm', 'Va'); setparameter(kineticlawObj,'Km', 'Ka');

**5** To retrieve a parameter variable:

```
parameterObj3 = getparameters(kineticlawObj, 'Vm')
```

MATLAB returns:

SimBiology Parameter Array

Index: Name: Value: ValueUnits: 1 Va 1

parameterObj4 = getparameters (kineticlawObj, 'Km')

**See Also** addparameter, getspecies, setparameter

Purpose	Get 3-D sensitivity matrix from SimData array	
Syntax	[T, R, Outputs,	InputFactors] = getsensmatrix(simDataObj) InputFactors] = getsensmatrix(simDataObj, nputFactorNames)
Arguments	Τ	<i>T</i> is an m-by-1 array specifying time points for the sensitivity data in R.
	R	<pre>R is an m-by-n-by-p array of sensitivity data with times, outputs, and input factors corresponding to its first, second, and third dimensions respectively. R(:,i,j) is the time course for the sensitivity of state Outputs{i} to the input factor InputFactors{j}.</pre>
	Outputs	Name of the output factors, where output factors are the names of the states for which you want to calculate sensitivity.
	InputFactors	Name of the input factors, where input factors are the names of the states with respect to which you want to calculate sensitivity.
Description		<pre>InputFactors] = getsensmatrix(simDataObj) gets ty data from the SimData object (simDataObj).</pre>
	arguments are ce	<i>j</i> contains more than one element, the output ll arrays in which each cell contains data for the ment of <i>simDataObj</i> .
	contained in the S in a SimData obje set used during th configuration set. Guide documenta	ix method can only return sensitivity data that is SimData object. The sensitivity data that is logged ect is set at simulation time by the configuration ne simulation. This is typically the model's active See "Sensitivity Analysis" in the SimBiology User's tion for an explanation of how to set up a sensitivity the configuration set. Note in particular that the

sensitivity data R returned by getsensmatrix may be normalized, as specified at simulation time.

```
[T, R, Outputs, InputFactors] =
```

getsensmatrix(simDataObj,OutputNames,InputFactorNames) gets
sensitivity data for the outputs specified by OutputNames and the input
factors specified by InputFactorNames.

OutputNames and InputFactorNames can both be any one of the following:

- Empty array
- Single name
- Cell array of names

Pass an empty array for OutputNames or InputFactorNames to ask for sensitivity data on all output factors or input factors contained in simDataObj, respectively. You can also use qualified names such as 'CompartmentName.SpeciesName' or 'ReactionName.ParameterName' to resolve ambiguities.

# **Examples** This example shows how to retrieve sensitivity data from a SimData object.

- **1** Set up the simulation:
  - a Import the radio decay model from SimBiology demos.

modelObj = sbmlimport('radiodecay');

**b** Retrieve the configset object from the modelObj.

configsetObj = getconfigset(modelObj);

• Specify the species for which you want sensitivity data in the SpeciesOutputs property. All model species are selected in this example.

Use the sbioselect function to retrieve the species objects from the model.

```
set (configsetObj.SensitivityAnalysisOptions, 'SpeciesOutputs', ...
sbioselect(modelObj, 'Type', 'species'));
```

**d** Specify parameters and species with respect to which you want to calculate the sensitivities in the ParameterInputFactors and the SpeciesInputFactors properties respectively.

set(configsetObj.SensitivityAnalysisOptions,'ParameterInputFactors', ... sbioselect(modelObj, 'Type', 'parameter', 'Name', 'c'));

set(configsetObj.SensitivityAnalysisOptions,'SpeciesInputFactors', ... sbioselect(modelObj,'Type', 'species', 'Name', 'z'));

e Enable SensitivityAnalysis.

```
set(configsetObj.SolverOptions, 'SensitivityAnalysis', true)
get(configsetObj.SolverOptions, 'SensitivityAnalysis')
ans =
```

```
1
```

f Simulate and return the results in a SimData object.

simDataObj = sbiosimulate(modelObj)

- 2 Extract and plot sensitivity data from the SimData object.
  - **a** Use getsensmatrix to retrieve sensitivity data.

[t R outs ifacs] = getsensmatrix(simDataObj);

**b** Plot sensitivity values.

plot(t, R(:,:,2)); legend(outs); title(['Sensitivities of species relative to ' ifacs{2}]);

See Also display, get, getdata, resample, selectbyname MATLAB function struct

Purpose	Get specific species in kinetic law object	
Syntax	<pre>speciesObj = getspecies(kineticlawObj) speciesObj = getspecies(kineticlawObj,</pre>	
Arguments	kineticlawObj	Retrieve species used by the kinetic law object.
	SpeciesVariablesValue	Retrieve species used by the kinetic law object corresponding to the specified species in the SpeciesVariables property of the kinetic law object.
Description	<pre>speciesObj = getspecies(kineticlawObj) returns the species used by the kinetic law object kineticlawObj to speciesObj.</pre>	
	<pre>speciesObj = getspecies(kinetic returns the species in the Specie speciesObj.</pre>	clawObj, 'SpeciesVariablesValue') esVariableNames property to
	SpeciesVariablesValue is the n appears in the SpeciesVariables SpeciesVariablesValue can be a	s property of kineticlawObj.
	and model objects. If you change updates to use the new name. You applicable elements such as rules	reaction objects, kinetic law objects, the name of a species, the reaction u must, however, configure all other that use the species, and the kinetic s. Use the method setspecies to a.
Examples	Create a model, add a reaction, SpeciesVariableNames for the re 1 Create a model object, and the	eaction rate equation.

```
modelObj = sbiomodel('my model');
                        reactionObj = addreaction(modelObj, 'a -> c + d');
                   2 Create a kinetic law object for the reaction object, of the type
                     'Henri-Michaelis-Menten'.
                        kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
                     reactionObj KineticLaw property is configured to kineticlawObj.
                   3 The 'Henri-Michaelis-Menten' kinetic law has one species variable
                     (S) that should to be set. To set this variable:
                        setspecies(kineticlawObj,'S', 'a');
                   4 Retrieve the species variable using getspecies.
                        speciesObj = getspecies (kineticlawObj, 'S')
                     MATLAB returns:
                        SimBiology Species Array
                        Index: Compartment: Name: InitialAmount: InitialAmountUnits:
                           1
                                   unnamed
                                                а
                                                          0
See Also
                   addspecies, getparameters, setparameter, setspecies
```

Purpose	Get stoichiometry matrix from model object	
Syntax	<pre>M = getstoichmatrix(modelObj) M = getstoichmatrix(modelObj, 'flat') [M,objSpecies] = getstoichmatrix(modelObj) [M,objSpecies,objReactions] = getstoichmatrix(modelObj)</pre>	
Arguments	М	Adjacency matrix for <i>mode10bj</i> .
	modelObj	Specify the model object <i>modelObj</i> .
	'flat'	Return the stoichiometry matrix for only the specified <i>mode10bj</i> , not for objects contained in the <i>Obj</i> .
	objSpecies	Return the list of <i>modelObj</i> species by Name property of the species. If the species are in multiple compartments, species names are qualified with the compartment name in the form compartmentName.speciesName. For example, nucleus.DNA, cytoplasm.mRNA.
	objReactions	Return the list of <i>modelObj</i> reactions by the Name property of reactions.
Description	getstoichmatrix returns a stoi	chiometry matrix for a model object.
	M = getstoichmatrix(modelObj) returns a stoichiometry matrix for SimBiology model object (modelObj) to M.	
	A stoichiometry matrix is defined by listing all reactions contained by <i>modelObj</i> column-wise and all species contained by <i>modelObj</i> row-wise in a matrix. The species of the reaction are represented in the matrix with the stoichiometric value at the location of [row of species, column	

of reaction]. Reactants have negative values. Products have positive values. All other locations in the matrix are 0.

For example, if *modelObj* is a model object with two reactions with names R1 and R2 and Reaction values of 2 A + B -> 3 C and B + 3 D -> 4 A, the stoichiometry matrix would be defined as:

	А	В	С	D
R1	-2	- 1	3	0
R2	4	- 1	0	- 3

M = getstoichmatrix(modelObj, 'flat') defines the stoichiometry
matrix for only modelObj. M is the stoichiometry matrix for the reactions
and species contained by modelObj.

[M,objSpecies] = getstoichmatrix(modelObj) returns the stoichiometry matrix to M and the species to objSpecies. objSpecies is defined by listing all Name property values of species contained by Obj. In the above example, objSpecies would be {'A', 'B', 'C', 'D'};.

[M,objSpecies,objReactions] = getstoichmatrix(modelObj) returns the stoichiometry matrix to M and the reactions to objReactions. objReactions is defined by listing all Name property values of reactions contained by modelObj. In the above example, objReactions would be {'R1', 'R2'}.

**Examples** 1 Read in a model using sbmlimport.

modelObj = sbmlimport('lotka.xml');

2 Get the stoichiometry matrix for the modelObj.

```
[M,objSpecies,objReactions] = getstoichmatrix(modelObj)
```

**See Also** getadjacencymatrix

Purpose	Get variant from model	
Syntax	variantObj = getvariant(modelObj) variantObj = getvariant(modelObj, 'NameValue')	
Arguments	variantObj modelObj 'NameValue'	Variant object returned by the getvariant method. Model object from which to get the variant. Name of the variant to get from the model object modelObj.
Description	<pre>variantObj = getvariant(modelObj) returns SimBiology variant objects contained by the SimBiology model object modelObj to variantObj. A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see Variant object. variantObj = getvariant(modelObj, 'NameValue') returns the SimBiology variant object with the name NameValue, contained by the SimBiology model object, modelObj. View properties for a variant object with the get command, and modify properties for a variant object with the set command.</pre>	
		ect to another model, use copyobj. To remove a SimBiology model, use the delete method.

# getvariant (model)

Examples	<b>1</b> Create a model containing several variants.	
	<pre>modelObj = sbiomodel('mymodel'); variantObj1 = addvariant(modelObj, 'v1'); variantObj2 = addvariant(modelObj, 'v2');</pre>	
	<b>2</b> Get all variants in the model.	
	vObjs = getvariant(modelObj)	
	SimBiology Variant Array	
	Index: Name: Active:	
	1 v1 false	
2 v2 false 3 Get the variant object named 'v2' from the model		
See Also	addvariant, removevariant	

#### **Purpose** Kinetic law information for reaction

# **Description** The kinetic law object holds information about the abstract kinetic law applied to a reaction and provides a template for the reaction rate. In the model, the SimBiology software uses the information you provide in a fully defined kinetic law object to determine the ReactionRate property in the reaction object.

When you first create a kinetic law object, you must specify the name of the abstract kinetic law to use. The SimBiology software fills in the KineticLawName property and the Expression property in the kinetic law object with the name of the abstract kinetic law you specified and the mathematical expression respectively. The software also fills in the ParameterVariables property and the SpeciesVariables property of the kinetic law object with the values found in the corresponding properties of the abstract kinetic law object.

To obtain the reaction rate, you must fully define the kinetic law object:

- 1 In the ParameterVariableNames property, specify the parameters from the model that you want to substitute in the expression (Expression property).
- **2** In the SpeciesVariableNames property, specify the species from the model that you want to substitute in the expression.

The SimBiology software substitutes in the expression, the names of parameter variables and species variables in the order specified in the ParameterVariables and SpeciesVariables properties respectively.

The software then shows the substituted expression as the reaction rate in the ReactionRate property of the reaction object. If the kinetic law object is not fully defined, the ReactionRate property remains ' ' (empty).

For links to kinetic law object property reference pages, see "Property Summary" on page 4-100.

Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can interactively change object properties in the SimBiology desktop.

For an explanation of how relevant properties relate to one another, see "Command Line" on page 4-96.

The following sections use a kinetic law example to show how you can fully define your kinetic law object to obtain the reaction rate in the SimBiology desktop and at the command line.

The Henri-Michaelis-Menten kinetic law is expressed as follows:

$$V_{\rm m} * S / (K_m + S)$$

In the SimBiology software Henri-Michaelis-Menten is a built-in abstract kinetic law, where  $V_{\rm m}$  and  $K_{\rm m}$  are defined in the ParameterVariables property of the abstract kinetic law object, and S is defined in the SpeciesVariables property of the abstract kinetic law object.

#### SimBiology Desktop

To fully define kinetic law, in the SimBiology desktop, define the names of the species variables and parameter variables that participate in the reaction rate in the **Project Settings-Reactions** pane on the **Kinetic Law** tab. To add a reaction and set the reaction rate in the SimBiology desktop, see "Adding Reactions to a Model" in the SimBiology Getting Started Guide documentation.

#### **Command Line**

To fully define the kinetic law object at the command line, define the names of the parameters in the ParameterVariableNames property of the kinetic law object, and define the species names in the SpeciesVariableNames property of the kinetic law object. For example, to apply the Henri-Michaelis-Menten abstract kinetic law to a reaction

A -> B where Vm = Va, Km = Ka and S = A

Define Va and Ka in the ParameterVariableNames property to substitute the variables that are in the ParameterVariables property (Vm and Km). Define A in the SpeciesVariableName property to be used to substitute the species variable in the SpeciesVariables property (S). Specify the order of the model parameters to be used for substitution in the same order that the parameter variables are listed in the ParameterVariables property. Similarly, specify species order if more than one species variable is represented.

```
% Find the order of the parameter variables
% in the kinetic law expression.
get(kineticlawObj, 'ParameterVariables')
ans =
    'Vm' 'Km'
% Find the species variable in the
% kinetic law expression
get(kineticlawObj, 'SpeciesVariables')
ans =
    'S'
% Specify the parameters and species variables
% to be used in the substitution.
% Remember to specify order, for example Vm = Va
% Vm is listed first in 'ParameterVariables',
% therefore list Va first in 'ParameterVariableNames'.
set(kineticlawObj,'ParameterVariableNames', {'Va' 'Ka'});
set(kineticlawObj,'SpeciesVariableNames', {'A'});
```

The rate equation is assigned in the reaction object as follows:

Va\*A/(Ka + A)

For a detailed procedure, see "Examples" on page 4-101.

The following table summarizes the relationships between the properties in the abstract kinetic law object and the kinetic law object in the context of the above example.

Property	Property Purpose	Abstract Kinetic Law Object	Kinetic Law Object
Name (abstract kinetic law object) KineticLawName (kinetic law object)	Name of abstract kinetic law applied to a reaction. For example: Henri-Michaelis -Menten	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only
Expression	Mathematical expression used to determine the reaction rate equation. For example: $V_{\rm m} * S / (K_m + S)$	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only; depends on abstract kinetic law applied to reaction.

Property	Property Purpose	Abstract Kinetic Law Object	Kinetic Law Object
ParameterVariables	Variables in Expression that are parameters. For example: Vm and Km	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only; depends on abstract kinetic law applied to reaction.
SpeciesVariables	Variables in Expression that are species. For example: S	Read-only for built-in abstract kinetic law. User-determined for user-defined abstract kinetic law.	Read-only; depends on abstract kinetic law applied to reaction.
ParameterVariableNames	Variables in ReactionRate that are parameters. For example: Va and Ka	Not applicable	Define these variables corresponding to ParameterVariables.
SpeciesVariablesNames	Variables in ReactionRate that are species. For example: A	Not applicable	Define these variables corresponding to SpeciesVariables.

Constructor Summary

addkineticlaw (reaction)

Create kinetic law object and add to reaction object

## KineticLaw object

Method Summary	addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	getparameters (kineticlaw)	Get specific parameters in kinetic law object
	getspecies (kineticlaw)	Get specific species in kinetic law object
	set (any object)	Set object properties
	setparameter (kineticlaw)	Specify specific parameters in kinetic law object
	setspecies (kineticlaw)	Specify species in kinetic law object
Property Summary	Annotation	Store link to URL or file
	Expression	Expression to determine reaction rate equation
	KineticLawName	Name of kinetic law applied to reaction
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parameters	Array of parameter objects

	ParameterVariableNames	Cell array of reaction rate parameters
	ParameterVariables	Parameters in abstract kinetic law
	Parent	Indicate parent object
	SpeciesVariableNames	Cell array of species used in reaction rate equation
	SpeciesVariables	Species in abstract kinetic law
	Tag	Specify label for SimBiology object
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object
Examples	This example shows how to defin	ne the reaction rate for a reaction.
	1 Create a model object, and a	dd a reaction object to the model.
	modelObj = sbiomodel ( reactionObj = addreact	'my_model'); ion (modelObj, 'A -> B');
	<b>2</b> Define a kinetic law for the re	eaction object.
	kineticlawObj = addkineticlaw	<pre>w(reactionObj, 'Henri-Michaelis-Menten');</pre>
	<b>3</b> Query the parameters and sp law.	ecies variables defined in the kinetic
	get(kineticlawObj, 'Pa	rameterVariables')
	ans =	
	'Vm' 'Km'	

```
get(kineticlawObj, 'SpeciesVariables')
ans =
    'S'
```

4 Define Va and Ka as ParameterVariableNames, which correspond to the ParameterVariables Vm and Km. To set these variables, first create the parameter variables as parameter objects (parameterObj1, parameterObj2) with the names Va and Ka, and then add them to kineticlawObj. The species object with Name A is created when reactionObj is created and need not be redefined.

```
parameterObj1 = addparameter(kineticlawObj, 'Va');
parameterObj2 = addparameter(kineticlawObj, 'Ka');
```

5 Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Va' 'Ka'});
set(kineticlawObj,'SpeciesVariableNames', {'A'});
```

**6** Verify that the reaction rate is expressed correctly in the reaction object ReactionRate property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

ans =

Va\*A/(Ka+A)

See Also AbstractKineticLaw object, Configset object, Model object, Parameter object, Reaction object, Root object, Rule object, Species object

SimBiology property Expression

Purpose	Model and componen	t information
---------	--------------------	---------------

# **Description** The SimBiology model object represents a *model*, which is a collection of interrelated reactions and rules that transform, transport, and bind species. The model includes model components such as compartments, reactions, parameters, rules, and events. Each of the components is represented as a property of the model object. A model object also has a default configuration set object to define simulation settings. You can also add more configuration set objects to a model object.

See "Property Summary" on page 4-105 for links to model property reference pages.

Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the SimBiology desktop.

You can retrieve top-level SimBiology model objects from the SimBiology root object. A SimBiology model object has its Parent property set to the SimBiology root object.

Constructor Summary	sbiomodel	Construct model object
Method Summary	addcompartment (model, compartment)	Create compartment object
	addconfigset (model)	Create configuration set object and add to model object
	addevent (model)	Add event object to model object
	addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
	addreaction (model)	Create reaction object and add to model object

## Model object

addrule (model)	Create rule object and add to model object
addvariant (model)	Add variant to model
copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
getadjacencymatrix (model)	Get adjacency matrix from model object
getconfigset (model)	Get configuration set object from model object
getstoichmatrix (model)	Get stoichiometry matrix from model object
getvariant (model)	Get variant from model
removeconfigset (model)	Remove configuration set from model
removevariant (model)	Remove variant from model
reorder (model, compartment)	Reorder component lists
set (any object)	Set object properties
setactiveconfigset (model)	Set active configuration set for model object
verify (model, variant)	Validate and verify SimBiology model

## Model object

Property	Annotation	Store link to URL or file
Summary	Compartments	Array of compartments in model or compartment
	Events	Contain all event objects
	Models	Contain all model objects
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parameters	Array of parameter objects
	Parent	Indicate parent object
	Reactions	Array of reaction objects
	Rules	Array of rules in model object
	Тад	Specify label for SimBiology object
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object

See Also AbstractKineticLaw object, Configset object, KineticLaw object, Parameter object, Reaction object, Root object, Rule object, Species object

Purpose	Parameter and scope information	
Description	The parameter object represents a <i>parameter</i> , which is a quantity that can change or can be constant. SimBiology parameters are generally used to define rate constants. You can add parameter objects to a model object or a kinetic law object. The scope of a parameter depends on where you add the parameter object: If you add the parameter object to a model object, the parameter is available to all reactions in the model and the Parent property of the parameter object is SimBiology.Model. If you add the parameter object to a kinetic law object, the parameter is available only to the reaction for which you are using the kinetic law object and the Parent property of the parameter object is SimBiology.KineticLaw.	
	See "Property Summary" on page 4 property reference pages.	-107 for links to parameter object
	Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.	
Constructor Summary	addparameter (model, kineticlaw)	Create parameter object and add to model or kinetic law object
Method Summary	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties

	rename (compartment, parameter, species)	Rename object and update expressions
	set (any object)	Set object properties
Property Summary	Annotation ConstantValue	Store link to URL or file Specify variable or constant parameter value
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Тад	Specify label for SimBiology object
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object
	Value	Assign value to parameter object
	ValueUnits	Parameter value units
See Alco	AbatasatKinatialaw abiast	Configurat object Kingticlaw

See Also AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Reaction object, Root object, Rule object, Species object

# **Reaction object**

Purpose	Options for model reactions	
Description	The reaction object represents a <i>reaction</i> , which describes a transformation, transport, or binding process that changes one or more species. Typically, the change is the amount of a species. For example:	
	Creatine + ATP <-> ADP +	phophocreatine
	glucose + 2 ADP + 2 Pi ->	2 lactic acid + 2 ATP + 2 H20
	Spaces are required before and after values.	er species names and stoichiometric
	See "Property Summary" on page 4 property reference pages.	4-109 for links to reaction object
	Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.	
Constructor Summary	addreaction (model)	Create reaction object and add to model object
Method Summary	addkineticlaw (reaction)	Create kinetic law object and add to reaction object
	addproduct (reaction)	Add product species object to reaction object
	addreactant (reaction)	Add species object as reactant to reaction object
	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object

	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	rmproduct (reaction)	Remove species object from reaction object products
	rmreactant (reaction)	Remove species object from reaction object reactants
	set (any object)	Set object properties
_		
Property Summary	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	KineticLaw	Show kinetic law used for ReactionRate
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Products	Array of reaction products
	Reactants	Array of reaction reactants
	Reaction	Reaction object reaction
	ReactionRate	Reaction rate equation in reaction object
	Reversible	Specify whether reaction is
		reversible or irreversible

Tag	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object
AbstractKineticLaw obi	ect.Configset object.KineticLaw

See Also AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Parameter object, Root object, Rule object, Species object

Purpose	Remove configuration set f	rom model
Syntax	removeconfigset( <i>modelObj</i> , removeconfigset( <i>modelObj</i> ,	
Arguments	modelObj NameValue configsetObj	Model object from which to remove the configuration set. Name of the configuration set. Configuration set object that is to be removed from the model object.
Description	removeconfigset(modelObj, 'NameValue') removes the configset object with the name NameValue from the SimBiology model object modelObj. A configuration set object stores simulation-specific information. A SimBiology model can contain multiple configuration sets with one being active at any given time. The active configuration set contains the settings that are used during the simulation. modelObj always contains at least one configuration set object with name configured to 'default'. You cannot remove the default configuration set from modelObj. If the active configuration set is removed from modelObj, then the default configuration set will be made active.	
	set object, configsetObj, f	<i>configsetObj</i> ) removes the configuration rom the SimBiology model, <i>modelObj</i> . The eted; if you want to delete configsetObj, use
		TLAB variable holding the configset, <i>j</i> , ' <i>NameValue</i> ') removes the configset it.
Examples	add a configset.	<pre>r importing the file oscillator.xml and port('oscillator');</pre>

	<pre>configsetObj = addconfigset(modelObj, 'myset');</pre>
	<b>2</b> Remove the configset from modelObj by name or alternatively by indexing.
	<pre>% Remove the configset with name 'myset'.     removeconfigset(modelObj, 'myset');</pre>
	<pre>% Get all configset objects and remove the second. configsetObj = getconfigset(modelObj); removeconfigset(modelObj, configsetObj(2));</pre>
See Also	addconfigset, getconfigset, setactiveconfigset

Purpose	Remove variant from model		
Syntax	-	variant(modelObj, 'NameValue') variant(modelObj, variantObj)	
Arguments	modelObj variantObj	Specify the model object from which you want to remove the variant. Specify the variant object to return from the model object.	
Description	<pre>variantObj = removevariant(modelObj, 'NameValue') removes a SimBiology variant object with the name NameValue from the model object modelObj and returns the variant object to variantObj. The variant object Parent property is assigned [] (empty). A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see Variant object.</pre>		
	<ul> <li>variantObj = removed</li> <li>SimBiology variant of</li> <li>variantObj.</li> <li>To view the variants</li> <li>method. To copy a variant</li> </ul>	variant(modelObj, variantObj) removes a oject (variantObj) and returns the variant object stored on a model object, use the getvariant riant object to another model, use copyobj. To add SimBiology model, use the addvariant method.	
Examples	modelObj = sb: variantObj1 = variantObj2 =	taining several variants. iomodel('mymodel'); addvariant(modelObj, 'v1'); addvariant(modelObj, 'v2'); addvariant(modelObj, 'v3'); object using its name.	

```
3 Remove a variant object using its index number.
a Get the index number of the variant in the model.
vObjs = getvariant(modelObj)
SimBiology Variant Array
Index: Name: Active:
1 v2 false
2 v3 false
```

removevariant(modelObj, 'v1');

**b** Remove the variant object.

removevariant(modelObj, vObjs(2));

See Also addvariant, getvariant

Purpose	Rename object and update expressions			
Syntax	rename(Obj, 'NewNameValue')			
Arguments	ObjCompartment, parameter, or species object.'NewNameValue'Specify the new name.			
Description	<pre>rename(Obj, 'NewNameValue'), changes the Name property of the object, Obj to NewNameValue and updates any expressions in the model (such as Rule or ReactionRate) to use the new name. If the new name is already being used by another model component, the new name will be qualified to ensure that it is unique. For example if you change a species named A to K, and a parameter with the name K exists, the species will be qualified as CompartmentName.K to indicate that the reference is to the species. If you are referring to an object by it's qualified name, for example CompartmentName.A and you change the species name, the reference will contain the qualified name in it's updated form, for example, CompartmentName.K</pre>			
Examples	<pre>changes the Name property of the object, except for species objects where the species object's Name property and any reaction strings which refer to species are updated to use the new name. 1 Create a model object that contains a species A in a rule.     m = sbiomodel('cell');</pre>			
	<pre>s = addspecies(m, 'A'); r = addrule(m, 'A = 4'); 2 Rename the species to Y rename(s, 'Y');</pre>			

## rename (compartment, parameter, species)

**3** See that the rule expression is now updated.

r

set

SimBiology Rule Array

Index:	RuleType:	Rule:
1	initialAssignment	Y = 4

See Also

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Purpose	Reorder component lists			
Syntax	<i>modelObj</i> = reorder(	Obj, NewOrder)		
Arguments	<i>Obj</i> Model object or compartment. Enter a vari name.			
	NewOrder	Object vector in the new order. If <i>Obj</i> is a model object, <i>NewOrder</i> can be an array of compartments, events, parameters, reactions or rules objects. If <i>Obj</i> is a compartment object, <i>NewOrder</i> must be an array of species objects.		
Description	<pre>modelObj = reorder(Obj, NewOrder) reorders the component vector NewOrder, to be in the order specified.</pre>			
	You can use this method to reorder any of the component vectors, such as events, parameters, rules, and species. The vector of components, when reordered, must contain the same objects as the original list of objects but they can be in a different order.			
Examples	I Import a model.			
	<pre>modelObj = sbmlimport('lotka');</pre>			
	<b>2</b> Display the order of the reactions in the model.			
	<pre>get(modelObj.Reactions);</pre>			
	SimBiology Reaction Array			
	Index: 1 2 3	Reaction: x + y1 -> 2 y1 + x y1 + y2 -> 2 y2 y2 -> z		

**3** Reverse the order of the reactions in the model.

reorder(modelObj, modelObj.Reactions([3 2 1]))

Purpose	Resample SimData object array onto new time vector		
Syntax	<pre>newSimDataObj = resample(simDataObj) newSimDataObj = resample(simDataObj, timevector) newSimDataObj = resample(simDataObj, timevector, method)</pre>		
Arguments	newSimDataObj simDataObj timevector method	<ul> <li>Resampled SimData object array.</li> <li>SimData object array that you want to resample.</li> <li>Real numeric array of time points onto which you want to resample the data.</li> <li>Method to use during resampling. Can be one of the following:</li> <li>'interp1q' — Uses the MATLAB function interp1, specify one of the following methods: <ul> <li>'nearest'</li> <li>'linear'</li> <li>'pchip'</li> <li>'cubic'</li> <li>'zoh' — specifies zero-order hold.</li> </ul> </li> </ul>	
Description	-	resample( <i>simDataObj</i> ) resamples the simulation data	

scriptionnewSimDataObj = resample(simDataObj) resamples the simulation data<br/>contained in every element of the SimData object array simDataObj onto<br/>a common time vector, producing a new SimData array newSimDataObj.<br/>By default, the common time vector is taken from the element of<br/>simDataObj with the earliest stopping time.

newSimDataObj = resample(simDataObj, timevector) resamples
the SimData array simDataObj onto the time vector timevector.
timevector must either be a real numeric array or the empty array
[]. If you use an empty array, resample uses the default time vector
as described above.

newSimDataObj = resample(simDataObj, timevector, method) uses the
interpolation method specified in method.

If the specified *timevector* includes time points outside the time interval encompassed by one or more SimData objects in *simDataObj*, the resampling will involve extrapolation and you will see a warning. See the help for the MATLAB function corresponding to the interpolation method in use for information on how the function performs the extrapolation.

#### Examples Simulating and Resampling Data

1 The project file, radiodecay.sbproj contains a model stored in a variable called m1. Load m1 into the MATLAB workspace.

```
sbioloadproject('radiodecay');
simDataObj = sbiosimulate(m1);
```

**2** Resample the data.

newSimDataObj = resample(simDataObj, [1:5], 'linear');

#### **Resampling Data for Ensemble Runs**

1 The project file, radiodecay.sbproj, contains a model stored in a variable called m1. Load m1 into the MATLAB workspace.

sbioloadproject('radiodecay');

**2** Change the solver to use during the simulation and perform an ensemble run.

csObj = getconfigset(m1);

	set(csObj, 'SolverType', 'ssa'); simDataObj = sbioensemblerun(m1, 10);
	<b>3</b> Interpolate the time steps.
	<pre>newSimDataObj = resample(simDataObj, [1:10], 'linear');</pre>
	<b>4</b> View the time steps in the SimData object arrays.
	newSimDataObj(1).Time simDataObj(1).Time
See Also	sbioensemblerun, sbioensemblestats, sbiosimulate, SimData object
	MATLAB functions interp1, interp1q

## reset (root)

Purpose	Delete all model objects from root object			
Syntax	reset(sbioroot)			
Description	reset(sbioroot) deletes all SimBiology model objects contained by the SimBiology root. The SimBiology root object is returned with the method sbioroot. This call is equivalent to sbioreset.			
	The SimBiology root object contains a list of SimBiology model objects, available units, unit prefixes, and abstract kinetic law objects. A SimBiology model object has its Parent property set to the SimBiology root object.			
	To add an abstract kinetic law to the SimBiology root user-defined library, use the sbioaddtolibrary function. To add a unit to the SimBiology root user-defined library, use the function sbioregisterunit. To add a unit prefix to the SimBiology root user-defined library, use the function sbioregisterunitprefix.			
Examples	l Query sbioroot, which has two model objects.			
	sbioroot			
	SimBiology Root Contains:			
	Models:	2		
	Builtin Abstract Kinetic Laws:	3		
	User Abstract Kinetic Laws:	1		
	Builtin Units:	54		
	User Units:	0		
	Builtin Unit Prefixes:	13		
	User Unit Prefixes:	0		
	<b>2</b> Call reset.			
	sbioroot			
	SimBiology Root Contains:			

Models:	0
Builtin Abstract Kinetic Laws:	3
User Abstract Kinetic Laws:	1
Builtin Units:	54
User Units:	0
Builtin Unit Prefixes:	13
User Unit Prefixes:	0

See Also sbioaddtolibrary, sbiohelp, sbioregisterunit, sbioregisterunitprefix, sbioreset, sbioroot

Purpose	Remove contents from variant object		
Syntax	rmcontent(variantObj, contents) rmcontent(variantObj, idx)		

#### Arguments

variantObj Specify the variant object from which you want to remove data. The Content property is modified to remove the new data.

contents Specify the data you want to remove from a variant object. Contents
can either be a cell array or an array of cell arrays. A valid cell
array should have the form {'Type', 'Name', 'PropertyName',
PropertyValue}, where PropertyValue is the new value to be
applied for the PropertyName. Valid Type, Name, and PropertyName
values are as follows.

′Туре′	'Name'	'PropertyName'
'species'	Name of the species. If there are multiple species in the model with the same name, specify the species as [compartmentName.speciesName], where compartmentName is the name of the compartment containing the species.	'InitialAmount'
'parameter'	If the parameter scope is a model, specify the parameter name. If the parameter scope is a kinetic law, specify [reactionName.parameterName].	'Value'
'compartment'	Name of the compartment.	'Capacity'

idx

Specify the ContentIndex or indices of the data to be removed. To display the ContentIndex, enter the object name and press Enter.

**Description** rmcontent(variantObj, contents) removes the data stored in the variable contents from the variant object (variantObj).

rmcontent(variantObj, idx) removes the data specified by the indices idx (also called ContentIndex) from the Content property of the variant object.

**Examples** 1 Create a model containing three species in one compartment.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
A = addspecies(compObj, 'A');
B = addspecies(compObj, 'B');
C = addspecies(compObj, 'C');
```

2 Add a variant object that varies the species' InitialAmount property.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {{'species', 'A', 'InitialAmount', 5}, ...
{'species', 'B', 'InitialAmount', 10}, ...
{ 'species', 'C', 'InitialAmount', 15}});% Display the variant
variantObj
```

SimBiology Variant - v1 (inactive)

ContentIndex:	Type:	Name:	Property:	Value:
1	species	А	InitialAmount	5
2	species	В	InitialAmount	10
3	species	С	InitialAmount	15

**3** Use the ContentIndex number to remove a species from the Content property of the variant object.

```
rmcontent(variantObj, 2);
variantObj
```

SimBiology Variant - v1 (inactive)

ContentIndex:	Type:	Name:	Property:	Value:
1	species	A	InitialAmount	5
2	species	C	InitialAmount	15

**4** (Alternatively) Remove a species from the contents of the variant object using detailed reference to the species.

```
rmcontent(variantObj, {'species','A', 'InitialAmount', 5});
% Display variant object
variantObj
SimBiology Variant - v1 (inactive)
ContentIndex: Type: Name: Property: Value:
1 species C InitialAmount 15
```

**See Also** addvariant, rmcontent, sbiovariant

Purpose	Remove species object from reaction object products	
Syntax	rmproduct( <i>reactionObj</i> , SpeciesName) rmproduct( <i>reactionObj</i> , speciesObj)	
Arguments	reactionObj Reaction object.	
	SpeciesName	Reaction object. Name for a model object. Enter a species name or a cell array of species names.
	speciesObj	Species object. Enter a species object or an array of species objects.
Description	<pre>rmproduct(reactionObj, SpeciesName), in a reaction object (reactionObj), removes a species object with a specified name (SpeciesName) from the property Products, removes the species name from the property Reaction, and updates the property Stoichiometry to exclude the species coefficient.</pre>	
		<i>bj</i> , <i>species0bj</i> ) removes a species object as g a MATLAB variable for a species object.
	The species object is not removed from the parent model property Species. If the species object is no longer used by any reaction, you can use the function delete to remove it from the parent object.	
	If one of the species specified does not exist as a product, a warning is returned.	
Examples	Example 1	
	_	how to remove a product that was previously added n remove the species object using the species name.
	modelObj = sbiomode reactionObj = addre	l('cell'); action(modelObj, 'Phosphocreatine + ADP -> creatine + ATP + Pi');

rmproduct(reactionObj, 'Pi')

SimBiology Reaction Array Index: Reaction: 1 Phosphocreatine + ADP -> creatine + ATP

#### Example 2

Remove a species object using a model index to a species object.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'A -> B + C');
reactionObj.Reaction
ans =
        A -> B + C
rmproduct(reactionObj, modelObj.Species(2));
reactionObj.Reaction
        ans =
        A -> C
```

See Also rmreactant

Purpose	Remove species object from reaction object reactants	
Syntax	rmreactant( <i>reactionObj</i> , <i>SpeciesName</i> ) rmreactant( <i>reactionObj</i> , <i>speciesObj</i> )	
Arguments	reactionObj SpeciesName speciesObj	Reaction object. Name for a species object. Enter a species name or a cell array of species names. Species object. Enter a species object or an array of species objects.
Description	<pre>rmreactant(reactionObj, SpeciesName), in a reaction object (reactionObj), removes a species object with a specified name (SpeciesName) from the property Reactants, removes the species name from the property Reaction, and updates the property Stoichiometry to exclude the species coefficient. rmreactant(reactionObj, speciesObj) removes a species object as described above using a MATLAB variable for a species object, or a</pre>	
	<ul><li>model index for a species object.</li><li>The species object is not removed from the parent model property</li><li>Species. If the species object is no longer used by any reaction, you can</li><li>use the method delete to remove it from the parent object.</li><li>If one of the species specified does not exist as a reactant, a warning is returned.</li></ul>	
Examples	<pre>is returned. Example 1 This example shows how to remove a reactant that was added to a reaction by mistake. You can remove the species object using the species name. modelObj = sbiomodel('cell'); reactionObj = addreaction(modelObj, 'Phosphocreatine + ADP + Pi -&gt; creatine + ATP');</pre>	

rmreactant(reactionObj, 'Pi')
SimBiology Reaction Array
Index: Reaction:
1 Phosphocreatine + ADP -> creatine + ATP

#### Example 2

Remove a species object using a model index to a species object.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(modelObj, 'A -> B + C');
reactionObj.Reaction
ans =
        A + B -> C
rmreactant(reactionObj, modelObj.Species(1));
reactionObj.Reaction
ans =
        A -> C
```

See Also

delete, rmproduct

Purpose	Hold models, unit libraries, and abstract kinetic law libraries	
Description	The SimBiology root object contains a list of the top-level SimBiology model objects and SimBiology libraries. The components that the libraries contain are: all available units, unit prefixes, and available abstract kinetic law objects. There are two types of libraries: one contains components that are built in (BuiltinLibrary), and the other contains components that are user defined (UserdefinedLibrary).	
	You can retrieve top-level SimBiology model objects from the SimBiology root object. A SimBiology model object has its Parent property set to the SimBiology root object.	
	See "Property Summary" on page 4 reference pages.	-132 for links to root object property
	Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can interactively change object properties in the SimBiology desktop.	
Constructor Summary	sbioroot	Return SimBiology root object
Method Summary	copyobj (any object)	Copy SimBiology object and its children
	get (any object)	Get object properties
	reset (root) Delete all model objects from root object	
	set (any object) Set object properties	

## Root object

Property Summary	BuiltInLibrary Models	Library of built-in components Contain all model objects
	Туре	Display top-level SimBiology object type
	UserDefinedLibrary	Library of user-defined components
See Also	AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Parameter object, Reaction object, Rule object, Species object	

Purpose	Hold rule for species and parameters		
Description	The SimBiology rule object represents a <i>rule</i> , which is a mathematical expression that modifies a species amount or a parameter value. For a description of the types of SimBiology rules, see RuleType.		
	See "Property Summary" on page - reference pages.	4-133 for links to rule property	
	Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.		
Constructor Summary	addrule (model)	Create rule object and add to model object	
Method Summary	copyobj (any object)	Copy SimBiology object and its children	
	delete (any object)	Delete SimBiology object	
	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	
	set (any object)	Set object properties	
Property Summary	Active	Indicate object in use during simulation	
	Annotation	Store link to URL or file	
	Name	Specify name of object	

Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rule	Specify species and parameter interactions
RuleType	Specify type of rule for rule object
Tag	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

See Also AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Species object

Purpose	Select data from SimData object	
Syntax	[t,x,names] = select(simDataObj, Query) [Out] = select(simDataObj, Query, 'Format', 'FormatValue')	
Arguments	Output Arguments	
	t	An n-by-1 vector of time points.
	X	An $n-by-m$ data array. $t$ and <i>names</i> label the rows and columns of $x$ respectively.
	names	An m-by-1 cell array of names.
	Out	Data returned in the format specified in 'FormatValue', shown in "Input Arguments" on page 4-135. Depending on the specified 'FormatValue', Out contains one of the following:
		• Structure array
		• SimData object
		• Time series object
		<ul> <li>Combined time series object from an array of SimData objects</li> </ul>

#### **Input Arguments**

simDataObj	SimData object array. Enter a variable name for a SimData object.
------------	---

```
Query A cell array of arguments consisting of some combination of property
name/property value pairs and/or 'Where' clauses. For a more
complete description of the query syntax, including 'Where' clauses
and their supported condition types, see sbioselect. You can use any
of the metadata fields available in the cells of the DataInfo property of
a SimData object in a query. These include 'Type', 'Name', 'Units',
'Compartment' (species only), or 'Reaction' (parameter only).
```

*FormatValue* Choose a format from the following table.

FormatValue	Description
'num'	Specifies the format that lets you return data in numeric arrays. This is the default when <b>select</b> is called with multiple output arguments.
'nummetadata'	Specifies the format that lets you return a cell array of metadata structures in <i>metadata</i> instead of names. The elements of <i>metadata</i> label the columns of $x$ .
'numqualnames'	Specifies the format that lets you return qualified names in <i>names</i> to resolve ambiguities.
'struct'	Specifies the format that lets you return a structure array holding both data and metadata. This is the default when you use a single output argument.
'simdata'	Specifies the format that lets you return data in a new SimData object. This is the default format when select is called with zero or one output argument.
'ts'	Specifies the format that lets you return data in time series objects, creating an individual time series for each state or column and SimData object in simDataObj.
'tslumped'	Specifies the format that lets you return data in time series objects, combining data from each SimData object into a single time series.

Description	<pre>[t,x,names] = select(simDataObj, Query) returns simulation time and state data from the SimData object (simDataObj) that matches the query argument Query.</pre>
	In a SimData object <i>simDataObj</i> , the columns of the data matrix simDataObj.Data are labeled by the cell array of metadata structures given by simDataObj.DataInfo. The select method enables you to pick out columns of the data matrix based on their metadata labels. For example, to extract data for all parameters logged in a SimData object <i>simDataObj</i> , use the syntax [ <i>t</i> , <i>x</i> , <i>names</i> ] = select ( <i>simDataObj</i> , {'Type', 'parameter'}].
	[Out] = select(simDataObj, Query, 'Format', 'FormatValue') returns the data in the specified format. Valid formats are listed in "Input Arguments" on page 4-135.
Examples	This example shows how to extract data of interest from your simulation data with the select method.
	1 The project file radiodecay.sbproj contains a model stored in a variable called m1. Load m1 into the MATLAB workspace.
	sbioloadproject gprotein_norules m1
	<b>2</b> Change the solver to use during the simulation and perform an ensemble run.
	csObj = getconfigset(m1); set(csObj, 'SolverType', 'ssa'); simDataObj = sbioensemblerun(m1, 10);
	<b>3</b> Select all species data logged in the SimData array sdarray.
	<pre>[t x n] = select(simDataObj, {'Type','species'});</pre>
	<b>4</b> Select data for the parameters with name 'Kd' and return the results in a new SimData object array.
	<pre>newsd = select(simDataObj, {'Type','parameter','name', 'Kd'});</pre>

	<b>5</b> This selects all data from simDataObj with a name that matches the pattern 'G' and returns time series objects.	
	<pre>ts = select(simDataObj, {'Where','Name','regexp','G'}, 'Format','ts');</pre>	
See Also	getdata, sbioselect, sbiosimulate, selectbyname, Simdata object	

Purpose	Select data by name from SimData object array		
Syntax	[ <i>t,x,n</i> ] = selectbyname( <i>simDataObj</i> , ' <i>NameValue</i> ') <i>Out</i> = selectbyname( <i>simDataObj</i> , <i>NameValue</i> , 'Format', <i>Format</i> )		
Arguments	Output Arguments		
	t	An n-by-1 vector of time points.	
	x	An n-by-m data array. <i>t</i> and <i>names</i> label the rows and columns of <i>x</i> respectively.	
	п	An m-by-1 cell array of names.	
	Out	<ul> <li>Data returned in the format as specified in <i>'FormatValue'</i>, shown in "Input Arguments" on page 4-139. Depending on the specified <i>'FormatValue'</i>, <i>Out</i> contains one of the following:</li> <li>Structure array</li> </ul>	
		• SimData object	
		• Time series object	
		<ul> <li>Combined time series object from an array of SimData objects</li> </ul>	
	Input Arguments		
	simDataObj	SimData object array. Enter a variable name for a SimData object.	
	Name Value Names of the states for which you want to		

Name Value Names of the states for which you want to select data from *simDataObj*. Must be either a string or a cell array of strings.

Query A cell array of arguments consisting of some combination of property name/property value pairs and/or 'Where' clauses. For a more complete description of the query syntax, including 'Where' clauses and their supported condition types, see sbioselect. You can use any of the metadata fields available in the cells of the DataInfo property of a SimData object. These include 'Type', 'Name', 'Units', 'Compartment' (species only), or 'Reaction' (parameter only).

FormatValue Choose a format from the following table.

FormatValue	Description
'num'	Specifies the format that lets you return data in numeric arrays. This is the default when select is called with multiple output arguments.
'nummetadata'	Specifies the format that lets you return a cell array of metadata structures in <i>metadata</i> instead of names. The elements of <i>metadata</i> label the columns of $x$ .
'numqualnames'	Specifies the format that lets you return qualified names in <i>names</i> to resolve ambiguities.
'struct'	Specifies the format that lets you return a structure array holding both data and metadata. This is the default when you use a single output argument.
'simdata'	Specifies the format that lets you return data in a new SimData object. This is the default format when select is called with zero or one output argument.

FormatValue	Description	
'ts'	Specifies the format that lets you return data in time series objects, creating an individual time series for each state or column and SimData object in simDataObj.	
'tslumped'	Specifies the format that lets you return data in time series objects, combining data from each SimData object into a single time series.	

### Description

The selectbyname method allows you to select data from a SimData object array by name. [t,x,n] = selectbyname(simDataObj, 'NameValue') returns time and state data from the SimData object simDataObj for states with names 'NameValue'.

In a SimData object *simDataObj*, the names labeling the columns of the data matrix *simDataObj*.Data are given by *simDataObj*.DataNames. A name specified in 'NameValue' can match more than one data column, for example, when *simDataObj* contains data for a species and parameter both named 'k'. To resolve ambiguities, use qualified names in 'NameValue', such as 'CompartmentName.SpeciesName' or 'ReactionName.ParameterName'. selectbyname returns qualified names in the output argument names when there are ambiguities.

Out = selectbyname(simDataObj, NameValue, 'Format', Format)
returns the data in the specified format. Valid formats are listed in
"Input Arguments" on page 4-139.

Examples % Get data for the species 'glucose' from the simdata array sdarray. [t x n] = selectbyname(sdarray,'glucose'); % Get data for multiple states and return the results in a struct array. s = selectbyname(sdarray,{'RexGFP';'nuc.GFP';'cytosol.GFP'},... 'Format','struct');

### See Also getdata, sbioselect, sbiosimulate

## set (any object)

Purpose	Set object properties		
Syntax	set(Obj, 'PropertyName', PropertyValue) set(Obj, 'PropertyName1', PropertyValue1, 'PropertyName2', PropertyValue2)		
Arguments	<i>Obj</i> Abstract kinetic law, compartment, configuration set, event, kinetic law, model, parameter, reaction, rule, species, or variant object.		
	'PropertyName'	Name of the property to set. For properties that you can set for each object, see AbstractKineticLaw object, Configset object, KineticLaw object, Model object, Parameter object, Reaction object, Rule object, Species object, Variant object	
	PropertyValue	Specify the value to set. Property values depend on the property being set. See the reference page for an object property for values that can be specified.	
Description	<pre>set(Obj, 'PropertyName', PropertyValue) sets the property 'PropertyName' of the object Obj, to PropertyValue.</pre>		
	<pre>set(Obj, 'PropertyName1', PropertyValue1, 'PropertyName2', PropertyValue2) sets the properties 'PropertyName1' and 'PropertyName2' to PropertyValue1 and PropertyValue2 respectively, and so on in sequence. You can specify multiple PropertyName, PropertyValue pairs.</pre>		
	When you want to change the name of a compartment, parameter, or species object, use the rename method instead of set. The rename method allows you to change the name and update the expressions in which these components are used. Whereas set only changes the Name property of the object, except for species objects where the species object's Name property and any reaction strings which refer to species are updated to use the new name.		

```
Examples 1 Create a model object.
    modelObj = sbiomodel ('my_model');
2 Add parameter object.
    parameterObj = addparameter (modelObj, 'kf');
3 Set the ConstantValue property of the parameter object to false
    and verify.
    MATLAB returns 1 for true and 0 for false.
    set (parameterObj, 'ConstantValue', false);
    get(parameterObj, 'ConstantValue')
    MATLAB returns
    ans =
        0
See Also
get, rename, setactiveconfigset
```

# setactiveconfigset (model)

Set active configuration set for model object		
configsetObj = setactiveconfigset(modelObj, 'NameValue') configsetObj2 = setactiveconfigset(modelObj, configsetObj1)		
<pre>configsetObj = setactiveconfigset(modelObj, 'NameValue') sets the configuration set NameValue to be the active configuration set for the model modelObj and returns to configsetObj.</pre>		
<pre>configsetObj2 = setactiveconfigset(modelObj, configsetObj1) sets the configset configsetObj1 to be the active configset for modelObj and returns to configsetObj2. Any change in one of these two configset objects configsetObj1 and configsetObj2 is reflected in the other. To copy over a configset object from one model object to another, use the copyobj method.</pre>		
The active configuration set contains the settings that are be used during a simulation. A default configuration set is attached to any new model.		
1 Create a model object by importing the file oscillator.xml and add a configset that simulates for 3000 seconds.		
<pre>modelObj = sbmlimport('oscillator'); configsetObj = addconfigset(modelObj, 'myset');</pre>		
<b>2</b> Configure the configsetObj StopTime to 3000.		
set(configsetObj, 'StopTime', 3000) get(configsetObj)		
Active: O CompileOptions: [1x1 SimBiology.CompileOptions] Name: 'myset' Notes: '' RuntimeOptions: [1x1 SimBiology.RuntimeOptions] SolverOptions: [1x1 SimBiology.ODESolverOptions]		

```
SolverType: 'ode15s'

StopTime: 3000

StopTimeType: 'simulationTime'

TimeUnits: 'second'

Type: 'configset'

3 Set the new configset to be active, simulate the model using the

new configset, and plot the result.

setactiveconfigset(modelObj, configsetObj);

[t,x] = sbiosimulate(modelObj);

plot (t,x)

See Also addconfigset, getconfigset, removeconfigset
```

# setparameter (kineticlaw)

Purpose	Specify specific parameters in kinetic law object		
Syntax	setparameter( <i>kineticlawObj</i> , 'ParameterVariablesValue', 'ParameterVariableNamesValue')		
Arguments	ParameterVariableValue ParameterVariableNamesValue	Specify the value of the parameter variable in the kinetic law object. Specify the parameter name with which to configure the parameter variable in the kinetic law object. Determines parameters in the	
Description	ReactionRate equation. Configure ParameterVariableNames in the kinetic law object. setparameter(kineticlawObj, 'ParameterVariablesValue', 'ParameterVariableNamesValue') configures the ParameterVariableNames property of the kinetic law object (kineticlawObj). ParameterVariableValue corresponds to one of the strings in kineticlawObj ParameterVariables property. The corresponding element in the kineticlawObjParameterVariableNames property is configured to ParameterVariableNamesValue. For example, if ParameterVariables is {'Vm', 'Km'} and ParameterVariablesValue is specified as Vm, then the first element of the ParameterVariableNames cell array is configured to ParameterVariableNamesValue.		
Examples	Create a model, add a reaction, and ParameterVariableNames for the rea 1 Create the model object, and then modelObj = sbiomodel('my_me	action rate equation. add a reaction object.	

```
reactionObj = addreaction(modelObj, 'a -> c + d');
                   2 Create a kinetic law object for the reaction object of the type
                      'Henri-Michaelis-Menten'.
                        kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
                     reactionObj KineticLaw property is configured to kineticlawObj.
                   3 The 'Henri-Michaelis-Menten' kinetic law has two parameter
                     variables (Vm and Km) that should be set. To set these variables:
                        setparameter(kineticlawObj,'Vm', 'Va');
                        setparameter(kineticlawObj,'Km', 'Ka');
                   4 Verify that the parameter variables are correct.
                        get (kineticlawObj, 'ParameterVariableNames')
                     MATLAB returns:
                        ans =
                             'Va'
                                     'Ka'
See Also
                   addparameter, getspecies, setspecies
```

# setspecies (kineticlaw)

Purpose	Specify species in kinetic law object		
Syntax	setspecies(kineticlawObj, 'SpeciesVariablesValue', 'SpeciesVariableNamesValue')		
Arguments	SpeciesVariablesValue	Specify the species variable in the kinetic law object.	
	SpeciesVariableNamesValue	Specify the species name with which to configure the species variable in the kinetic law object. Determines the species in the ReactionRate equation.	
Description	setspecies configures the kinetic law object SpeciesVariableNames property.		
	<pre>setspecies(kineticlawObj, 'SpeciesVariablesValue', 'SpeciesVariableNamesValue') configures the SpeciesVariableNames property of the kinetic law object, kineticlawObj. SpeciesVariablesValue corresponds to one of the strings in the SpeciesVariables property of kineticlawObj. The correspondin element in kineticlawObj SpeciesVariableNames property is configured to SpeciesVariableNamesValue. For example, if SpeciesVariables are {'S', 'S1'} and SpeciesVariablesValue is specified as S1, the first element of the SpeciesVariableNames cell array is configured to SpeciesVariableNamesValue.</pre>		
Examples	Create a model, add a reaction, and assign the SpeciesVariableNames for the reaction rate equation.		
	<pre>Create the model object, and th modelObj = sbiomodel('my reactionObj = addreactio</pre>	-	

**2** Create a kinetic law object for the reaction object of the type 'Henri-Michaelis-Menten'.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

reactionObj KineticLaw property is configured to kineticlawObj.

3 The 'Henri-Michaelis-Menten' kinetic law has one species variable (S) that should be set. To set this variable:

```
setspecies(kineticlawObj,'S', 'a');
```

**4** Verify that the species variable is correct.

```
get (kineticlawObj, 'SpeciesVariableNames')
```

MATLAB returns:

ans =

'a'

**See Also** addparameter, getspecies, setparameter

# SimData object

Purpose	Simulation data storage		
Description	The SimBiology SimData object contains simulation data. The output from the sbiosimulate function, is stored in the SimData object which holds time and state data as well as metadata, such as the types and names for the logged states or the configuration set used during simulation.		
	You can also store data from multiple simulation runs as an array of SimData objects. Thus, the output of sbioensemblerun is an array of SimData objects. You can use any SimData method on an array of SimData objects.		
	You can access the time, data, and metadata stored in the SimData object through the properties in "Property Summary" on page 4-151. Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line.		
	Methods you can use to query the SimData object are listed in "Method Summary" on page 4-150.		
Constructor Summary	sbioensemblerun	Multiple stochastic ensemble runs of SimBiology model	
	sbiosimulate	Simulate model object	
Method Summary	delete (any object) display (any object)	Delete SimBiology object Display summary of SimBiology object	
	get (any object)	Get object properties	
	getdata (SimData)	Get data from SimData object array	

	getsensmatrix (SimData)	Get 3-D sensitivity matrix from SimData array
	resample (SimData)	Resample SimData object array onto new time vector
	select (SimData)	Select data from SimData object
	selectbyname (SimData)	Select data by name from SimData object array
Property Summary	Data	Store simulation data
Sommary	DataCount	Numbers of species, parameters, sensitivities
	DataInfo	Metadata labels for simulation data
	DataNames	Show names in SimData object
	ModelName	Name of model simulated
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	RunInfo	Information about simulation
	Time	Show simulation time steps
	TimeUnits	Show stop time units for simulation
	UserData	Specify data to associate with object
See Also	AbstractKineticLaw object, Kin Parameter object, Reaction obj	

Species object

# **Species object**

Purpose	Options for compartment species		
Description	<ul> <li>The SimBiology species object represents a species, which is a chemical or entity that participates in reactions, for example, DNA, ATP, Pi, creatine, G-Protein, or Mitogen-Activated Protein Kinase (MAPK). Species amounts can vary or remain constant during a simulation.</li> <li>To add species that participate in reactions, add the reaction to the model. The process of adding the reaction to the model creates a compartment object (unnamed) and the necessary species objects.</li> <li>Alternatively, create and add a species object to a compartment object, using the addspecies method at the command line. The SimBiology desktop adds a default compartment (unnamed) for you and you can add a species in the Species pane. In the Project Explorer, expand Compartment and double-click Species to open the Species pane.</li> <li>See "Property Summary" on page 4-153 for links to species property reference pages. Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.</li> </ul>		
Constructor Summary	addspecies (compartment)	Create species object and add to compartment object	
Method	Methods for species objects		
Summary	copyobj (any object)	Copy SimBiology object and its children	
	delete (any object)	Delete SimBiology object	
	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	

	rename (compartment, parameter, species)	Rename object and update expressions
	set (any object)	Set object properties
Property Summary	Properties for species objects	
,	Annotation	Store link to URL or file
	BoundaryCondition	Indicate species boundary condition
	ConstantAmount	Specify variable or constant species amount
	InitialAmount	Species initial amount
	InitialAmountUnits	Species initial amount units
	Name	Specify name of object
	Notes	HTML text describing SimBiology object
	Parent	Indicate parent object
	Тад	Specify label for SimBiology object
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object
Saa Alca	Compositions shippt Configer	t object Kinstielew object Medel

# See Also Compartment object, Configset object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Rule object

# Unit object

Purpose	Hold information about user-defined unit		
Description	The SimBiology unit object holds information about user-defined units. To create a unit, create the unit object and add the unit to the library using the sbioaddtolibrary function.		
	Use the unit object property <b>Composition</b> to specify the composition of your units. See "Property Summary" on page 4-154 for links to unit object property reference pages.		
	Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at th command line. You can graphically change unit object properties us the <b>Unit Manager</b> in the SimBiology desktop.		
Constructor Summary	sbiounit	Create user-defined unit	
Method Summary	delete (any object) display (any object) get (any object) set (any object)	Delete SimBiology object Display summary of SimBiology object Get object properties Set object properties	
Property Summary	Annotation Composition Multiplier Name	Store link to URL or file Unit composition Relationship between defined unit and base unit Specify name of object	

Notes	HTML text describing SimBiology object
Offset	Unit composition modifier
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

See Also AbstractKineticLaw object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Rule object, Species object, UnitPrefix object

# UnitPrefix object

Purpose	Hold information about user-defined unit prefix		
Description	The SimBiology unit prefix object holds information about user-defined unit prefixes. To create a unit prefix, create the unit prefix object and add the unit prefix to the library using the sbioaddtolibrary function.		
	Use the unit prefix object property Exponent, to specify the expon of your unit prefix. See "Property Summary" on page 4-156 for lin unit prefix object property reference pages.		
	Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change unit prefix object properties using the <b>Unit Manager</b> in the SimBiology desktop.		
Constructor Summary	sbiounitprefix	Create user-defined unit prefix	
Method	delete (any object)	Delete SimBiology object	
Summary	display (any object)	Display summary of SimBiology object	
	get (any object)	Get object properties	
	set (any object)	Set object properties	
Property	Annotation	Store link to URL or file	
Summary	Exponent	Exponent value of unit prefix	
	Name	Specify name of object	
	Notes	HTML text describing SimBiology object	
	Parent	Indicate parent object	

	Тад	Specify label for SimBiology object
	Туре	Display top-level SimBiology object type
	UserData	Specify data to associate with object
See Also		oject, KineticLaw object, Model object,

AbstractKineticLaw object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Rule object, Species object, Unit object

### Variant object

#### **Purpose** Store alternate component values

**Description** The SimBiology variant object stores the names and values of model components and allows you to use the values stored in a variant object as the alternate value to be applied during a simulation. You can store values for species InitialAmount, parameter Value, and compartment Capacity in a variant object. Simulating using a variant does not alter the model component values. The values specified in the variant temporarily apply during simulation.

Using one or more variant objects associated with a model allows you to evaluate model behavior during simulation, with different values for the various model components without having to search and replace these values, or having to create additional models with these values. If you determine that the values in a variant object accurately define your model, you can permanently replace the values in your model with the values stored in the variant object, using the commit method.

To use a variant in a simulation you must add the variant object to the model object and set the Active property of the variant to true. Set the Active property to true if you always want the variant to be applied before simulating the model. You can also enter the variant object as an argument to sbiosimulate; this applies the variant only for the current simulation and supersedes any active variant objects on the model.

When there are multiple active variant objects on a model, if there are duplicate specifications for a property's value, the last occurrence for the property value in the array of variants, is used during simulation. You can find out which variant is applied last by looking at the indices of the variant objects stored on the model. Similarly, in the Content property, if there are duplicate specifications for a property's value, the last occurrence for the property in the Content property, is used during simulation.

Use the addcontent method to append contents to a variant object.

See "Property Summary" on page 4-159 for links to species property reference pages. Properties define the characteristics of an object. Use the get and set commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary	sbiovariant	Construct variant object
Method Summary	Methods for variant objects	
Sommary	addcontent (variant)	Append content to variant object
	commit (variant)	Commit variant contents to model
	copyobj (any object)	Copy SimBiology object and its children
	delete (any object)	Delete SimBiology object
	display (any object)	Display summary of SimBiology object
	get (any object)	Get object properties
	rmcontent (variant)	Remove contents from variant object
	set (any object)	Set object properties
	verify (model, variant)	Validate and verify SimBiology model
Property Summary	Properties for variant objects	
Johnnary	Active	Indicate object in use during simulation
	Annotation	Store link to URL or file
	Content	Contents of variant object
	Name	Specify name of object

Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

See Also Compartment object, Configset object, Model object, Parameter object, Species object

sbiosimulate

Purpose	Validate and verify SimBiology model	
Syntax	verify(modelObj) verify(modelObj, configsetObj) verify(modelObj, variantObj) verify(modelObj, configsetObj, variantObj)	
Description	<pre>verify(modelObj) performs checks on a model object (modelObj) to verify that you can simulate the model. This method generates stacked errors and warnings if any problems are found. To see the entire list of errors and warnings, use sbiolasterror and sbiolastwarning. The verify method uses the active configuration set for verification.</pre>	
	<pre>verify(modelObj, configsetObj) performs checks on the specified configuration set object (configsetObj) in conjunction with the model object (modelObj) to verify that you can simulate the model.</pre>	
	<pre>verify(modelObj, variantObj) performs checks on the variant object (variantObj) in conjunction with the model object (modelObj) to verify that you can simulate the model. The model object is required for the verification of the variant object.</pre>	
	<pre>verify(modelObj, configsetObj, variantObj) performs checks on the configuration set object configsetObj, and the variant object variantObj in conjunction with the model object (modelObj) to verify that you can simulate the model.</pre>	
	Verification in the SimBiology GUI	
	While you are building your model in the SimBiology desktop, you can click verify at any time to generate a list of any errors and warnings in the model. The errors and warnings appear in the <b>Errors and</b> <b>Warnings</b> pane.	
Examples	<pre>modelObj = sbmlimport('radiodecay.xml'); verify(modelObj);</pre>	
See Also	sbiolasterror, sbiolastwarning	

# **Property Reference**

Abstract Kinetic Law (p. 5-2) Properties for abstract kinetic law objects Compartments (p. 5-3) Properties for compartment objects Configuration Sets (p. 5-4) Properties for configuration set objects Events (p. 5-5)Properties for event objects Kinetic Laws (p. 5-6) Properties for kinetic law objects Models (p. 5-7) Properties for model objects Properties for parameter objects Parameters (p. 5-8) Reactions (p. 5-9) Properties for reaction objects Root (p. 5-10) Properties for the root object Rules (p. 5-11) Properties for rule objects Properties for SimData objects SimData (p. 5-12) Species (p. 5-13) Properties for species objects Unit (p. 5-13) Properties for unit objects Unit Prefix (p. 5-14) Properties for unit objects Properties for variant objects Variant (p. 5-14) Using Object Properties (p. 5-16) Command-line syntax for entering and retrieving property values

### Abstract Kinetic Law

Annotation	Store link to URL or file
Expression	Expression to determine reaction rate equation
Name	Specify name of object
Notes	HTML text describing SimBiology object
ParameterVariables	Parameters in abstract kinetic law
Parent	Indicate parent object
SpeciesVariables	Species in abstract kinetic law
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object $% \left( {{{\left( {{{{{\bf{b}}}} \right)}_{i}}}_{i}}} \right)$

## Compartments

Annotation	Store link to URL or file
Capacity	Compartment capacity
CapacityUnits	Compartment capacity units
Compartments	Array of compartments in model or compartment
ConstantCapacity	Specify variable or constant compartment capacity
Name	Specify name of object
Notes	HTML text describing SimBiology object
Owner	Owning compartment
Parent	Indicate parent object
Species	Array of species in compartment object
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

## **Configuration Sets**

Active	Indicate object in use during simulation
CompileOptions	Dimensional analysis and unit conversion options
Name	Specify name of object
Notes	HTML text describing SimBiology object
RuntimeOptions	Options for logged species
SensitivityAnalysisOptions	Specify sensitivity analysis options
SolverOptions	Specify model solver options
SolverType	Select solver type for simulation
StopTime	Set stop time for simulation
StopTimeType	Specify type of stop time for simulation
TimeUnits	Show stop time units for simulation
Туре	Display top-level SimBiology object type

#### Events

### **Events**

Active	Indicate object in use during simulation
Annotation	Store link to URL or file
EventFcns	Event expression
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Тад	Specify label for SimBiology object
Trigger	Event trigger
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

### **Kinetic Laws**

Annotation	Store link to URL or file
Expression	Expression to determine reaction rate equation
KineticLawName	Name of kinetic law applied to reaction
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parameters	Array of parameter objects
ParameterVariableNames	Cell array of reaction rate parameters
ParameterVariables	Parameters in abstract kinetic law
Parent	Indicate parent object
SpeciesVariableNames	Cell array of species used in reaction rate equation
SpeciesVariables	Species in abstract kinetic law
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

## **Models**

Annotation	Store link to URL or file
Compartments	Array of compartments in model or compartment
Events	Contain all event objects
Models	Contain all model objects
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parameters	Array of parameter objects
Parent	Indicate parent object
Reactions	Array of reaction objects
Rules	Array of rules in model object
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

### **Parameters**

Annotation	Store link to URL or file
ConstantValue	Specify variable or constant parameter value
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object
Value	Assign value to parameter object
ValueUnits	Parameter value units

## Reactions

Active	Indicate object in use during simulation
Annotation	Store link to URL or file
KineticLaw	Show kinetic law used for ReactionRate
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Products	Array of reaction products
Reactants	Array of reaction reactants
Reaction	Reaction object reaction
ReactionRate	Reaction rate equation in reaction object
Reversible	Specify whether reaction is reversible or irreversible
Stoichiometry	Species coefficients in reaction
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

### Root

BuiltInLibrary	Library of built-in components
Models	Contain all model objects
Туре	Display top-level SimBiology object type
UserDefinedLibrary	Library of user-defined components

## Rules

Active	Indicate object in use during simulation
Annotation	Store link to URL or file
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rule	Specify species and parameter interactions
RuleType	Specify type of rule for rule object
Tag	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

## SimData

Data	Store simulation data
DataCount	Numbers of species, parameters, sensitivities
DataInfo	Metadata labels for simulation data
DataNames	Show names in SimData object
ModelName	Name of model simulated
Name	Specify name of object
Notes	HTML text describing SimBiology object
RunInfo	Information about simulation
Time	Show simulation time steps
TimeUnits	Show stop time units for simulation
UserData	Specify data to associate with object

## **Species**

Annotation	Store link to URL or file
BoundaryCondition	Indicate species boundary condition
ConstantAmount	Specify variable or constant species amount
InitialAmount	Species initial amount
InitialAmountUnits	Species initial amount units
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

## Unit

Annotation	Store link to URL or file
Composition	Unit composition
Multiplier	Relationship between defined unit and base unit
Name	Specify name of object
Notes	HTML text describing SimBiology object
Offset	Unit composition modifier
Parent	Indicate parent object
Тад	Specify label for SimBiology object

Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

## **Unit Prefix**

Annotation	Store link to URL or file
Exponent	Exponent value of unit prefix
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

## Variant

Active	Indicate object in use during simulation
Annotation	Store link to URL or file
Content	Contents of variant object
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object

Тад	Specify label for SimBiology object
Туре	Display top-level SimBiology object type
UserData	Specify data to associate with object

### **Using Object Properties**

Command-line syntax for entering and retrieving property values.

Entering Property Values (p. 5-16)	Use either MATLAB functions or object dot notation to enter or change property values.
Retrieving Property Values (p. 5-16)	Use either MATLAB functions or object dot notation to get property values.
Help for Objects, Methods, and Properties (p. 5-17)	Use the command sbiohelp to get information about properties.

#### **Entering Property Values**

Enter or change a single property value using dot notation.

```
ObjectName.PropertyName = PropertyValue
```

Enter or change one or more property values using the MATLAB function set.

```
set(ObjectName, 'Propertyname', PropertyValue, ...)
```

#### **Retrieving Property Values**

Retrieve a single property value using dot notation.

PropertyValue = ObjectName.PropertyName

Retrieve one or more property values using the MATLAB function get.

```
PropertyValue(s) = get(ObjectName, 'PropertyName', ...)
```

Retrieve one or more property values using the object method get.

PropertyValue(s) = ObjectName.get('PropertyName', ...)

List or retrieve all property values using one of the following commands:

get(ObjectName)
AllPropertyValues = get(ObjectName)

ObjectName.get

#### Help for Objects, Methods, and Properties

Display information for SimBiology object methods and properties in the MATLAB Command Window.

help sbio	Display a list of functions and methods.
help FunctionName	Display function information.
<pre>sbiohelp('MethodName')</pre>	Display method information.
<pre>sbiohelp('PropertyName')</pre>	Display property information.

## Properties — Alphabetical List

## **AbsoluteTolerance**

**Purpose** Specify largest allowable absolute error

**Description** The AbsoluteTolerance property specifies the largest allowable absolute error at any step in simulation. It is a property of SolverOptions object. SolverOptions is a property of the configset object. AbsoluteTolerance is available for the ode solvers ('ode45', 'ode23', 'ode113', 'ode15s', 'ode23s', 'ode23t', and 'ode23tb').

At each simulation step, the solver estimates the local error  $e_i$  in the ith state vector y. Simulation converges at that time step if  $e_i$  satisfies the following equation:

 $|e_i| \le \max(\text{RelativeTolerance} * |y_i|, \text{AbsoluteTolerance})$ 

Thus at higher state values, convergence is determined by RelativeTolerance. As the state values approach zero, convergence is controlled by AbsoluteTolerance. The choice of values for RelativeTolerance and AbsoluteTolerance will vary depending on the problem. The default values should work for first trials of the simulation; however if you want to optimize the solution, consider that there is a trade-off between speed and accuracy. If the simulation takes too long, you can increase the values of RelativeTolerance and AbsoluteTolerance at the cost of some accuracy. If the results appear to be inaccurate, you can decrease the tolerance values but this will slow down the solver. If the magnitude of the state values is high, you can try to decrease the relative tolerance to get more accurate results.

This may be important for reactions where species values tend to zero. Even if you are not interested in the value of a state y(i) when it is small, you may have to specify AbsoluteTolerance small enough to get some correct digits in y(i) so that you can accurately compute more interesting state values.

#### **Characteristics**

Applies to	Object: SolverOptions
Data type	double

	Data values	>0, <1. Default is 1e-6.
	Access	Read/write
Examples	This example shows how to c	hange AbsoluteTolerance.
	1 Retrieve the configset of	oject from the modelObj.
	modelObj = sbiomode configsetObj = getco	
	<b>2</b> Change the AbsoluteTolerance to 1e-8.	
		LverOptions, 'AbsoluteTolerance', 1.0e-8); LverOptions, 'AbsoluteTolerance')
	ans =	
	1.0000e-008	
See Also	RelativeTolerance	

## Active

#### **Purpose** Indicate object in use during simulation

# **Description** The Active property indicates whether a simulation is using a SimBiology object. A SimBiology model is organized into a hierarchical group of objects. Use the Active property to include or exclude objects during a simulation.

- **Configuration set** For the configset object, use the method setactiveconfigset to set the object Active property to true.
- Event, Reaction, or Rule When an event, a reaction, or rule object Active property is set to false, the simulation does not include the event, reaction, or rule. This is a convenient way to test a model with and without a reaction or rule.
- Variant Set the Active property to true if you always want the variant to be applied before simulating the model. You can also pass the variant object as an argument to sbiosimulate; this applies the variant only for the current simulation. For more information on using the Active property for variants, see Variant object.

#### **Characteristics**

Applies to	Objects: configset, event, reaction, rule, or variant
Data type	boolean
Data values	true or false. The default value for events, reactions, and rules is true. For the configset object, default is true. For added configset object, the default is false. For variants, the default is false.
Access	Read/write

#### **Examples** 1 Create a model object.

modelObj = sbiomodel ('my\_model');

```
2 Add a reaction object and verify that the Active property setting
                    is 'true' or 1.
                       reactionObj = addreaction (modelObj, 'a + b -> c + d');
                       get (reactionObj, 'Active')
                    MATLAB returns:
                       ans =
                       1
                   3 Set the Active property to 'false' and verify.
                       set (reactionObj, 'Active', false);
                       get (reactionObj, 'Active')
                     MATLAB returns:
                       ans =
                       0
See Also
                  addconfigset, addreaction, addrule, Event object, Reaction
                  object, Rule object, setactiveconfigset, Variant object
```

## Annotation

Purpose	Store link to URL or file		
Description	The Annotation property stores the URL or file name linking to information about a model.		
Characteristics	Applies to	SimBiology objects: abstract kinetic law, configuration set, compartment, event, kinetic law, model, parameter, reaction, rule, species, or unit	
	Data type	char string, URL	
	Data values	Character string with a directory path and filename or a URL	
	Access	Read/write	
Examples	Create a model object.		
	<pre>modelObj = sbiomodel ('my_model');</pre>		
	<b>2</b> Set the annotation for a model object.		
	<pre>set (modelObj, 'annotation', 'www.reactome.org')</pre>		
	<b>3</b> Verify the assignment.		
	get (modelObj, 'annotation')		
	MATLAB returns:		
	ans =		
	www.reactome.c	org	
See Also	-	arameter, addreaction, addrule, addspecies, , sbiounit, sbiounitprefix	

#### **Purpose** Indicate species boundary condition

**Description** The BoundaryCondition property indicates whether a species object has a boundary condition. If BoundaryCondition is true, the species quantity is determined by InitialAmount and/or a rule object, and not by the reaction rate equation. All SimBiology species are state variables regardless of the BoundaryCondition or ConstantAmount property.

By default, BoundaryCondition is false and the reaction rate equations determine the rate of change of a species quantity in the model. Boundary condition is used when a species is modeled as a participant of reactions but the species quantity is not determined by a reaction rate equation.

#### **More Information**

Consider the following two use cases of boundary conditions:

• Modeling receptor-ligand interactions that affect the rate of change of the receptor but not the ligand. For example, in response to hormone, steroid receptors such as the glucocorticoid receptor (GR) translocate from the cytoplasm (cyt) to the nucleus (nuc). The hsp90/hsp70 chaperone complex directs this nuclear translocation [Pratt 2004]. The natural ligand for GR is cortisol; the synthetic hormone dexamethasone (dex) is used in place of cortisol in experimental systems. In this system dexamethasone participates in the reaction but the quantity of dexamethasone in the cell is regulated using a rule. To simply model translocation of GR you could use the following reactions:

Formation of the chaperone-receptor complex,

Hsp90\_complex + GR\_cyt -> Hsp90\_complex:GR\_cyt

In response to the synthetic hormone dexamethas one (dex), GR moves from the cytoplasm to the nucleus.

```
Hsp90_complex:GR_cyt + dex -> Hsp90_complex + GR_nuc + dex
```

For dex,

```
BoundaryCondition = true; ConstantAmount = false
```

In this example dex is modeled as a boundary condition with a rule to regulate the rate of change of dex in the system. Here, the quantity of dex is not determined by the rate of the second reaction but by a rate rule such as

ddex/dt = 0.001

which is specified in the SimBiology software as

dex = 0.001

• Modeling the role of nucleotides (for example, GTP, ATP, cAMP) and cofactors (for example, Ca<sup>++</sup>, NAD<sup>+</sup>, coenzyme A). Consider the role of GTP in the activation of Ras by receptor tyrosine kinases.

Ras-GDP + GTP -> Ras-GTP + GDP

For GTP, BoundaryCondition = true; ConstantAmount = true

Model GTP and GDP with boundary conditions, thus making them *boundary species*. In addition, you can set the ConstantAmount property of these species to true to indicate that their quantity does not vary during a simulation.

#### **Characteristics**

Applies to	Object: species
Data type	boolean
Data values	true or false. The default value is false.
Access	Read/write

**Examples** 1 Create a model object.

modelObj = sbiomodel ('my model');

```
2 Add a species object and verify that the boundary condition property
                     setting is 'false' or 0.
                        speciesObj = addspecies(modelObj, 'glucose');
                        get(speciesObj, 'BoundaryCondition')
                     MATLAB returns:
                        ans =
                             0
                   3 Set the boundary condition to 'true' and verify.
                        set(speciesObj, 'BoundaryCondition', true);
                        get(speciesObj, 'BoundaryCondition')
                     MATLAB returns:
                        ans =
                             1
References
                   Pratt, W.B., Galigniana, M.D., Morishima, Y., Murphy, P.J. (2004), Role
                   of molecular chaperones in steroid receptor action, Essays Biochem,
                   40:41-58.
See Also
                   addrule, addspecies, ConstantAmount, InitialAmount
```

## **BuiltInKineticLaws**

Purpose	Contain built-in kinetic	laws	
	<b>Note</b> BuiltInKineticL Use BuiltInLibrary in	aws has been removed and produces an error. stead.	
Description	BuiltInKineticLaws is a SimBiology root object property showing all abstract kinetic laws that are shipped with the SimBiology software. Use the command sbiowhos -builtin -kineticlaw to see the list of built-in kinetic laws. You can use built-in kinetic laws when you use the command addkineticlaw to create a kinetic law object for a reaction object. Refer to the kinetic law by name when you create the kinetic law object, for example:		
	kineticlawObj = ac	ldkineticlaw(reactionObj, 'Henri-Michaelis-Menten');	
	You cannot add, modify,	or delete BuiltInKineticLaws.	
	See "Abstract Kinetic Law" on page 6-49 for a definition and more information.		
Characteristics	6		
	Applies to	Object: root	
	Data type	char string of valid abstract kinetic law name	
	Data values	Valid kinetic laws	
	Access	Read-only	
See Also	BuiltInLibrary		

#### Purpose Library of built-in components

#### **Description** BuiltInLibrary is a SimBiology root object property containing all built-in components namely units, unit prefixes, and abstract kinetic laws that are shipped with the SimBiology product. You cannot add, modify, or delete components in the built-in library. The BuiltInLibrary property is an object that contains the following properties:

- Units Contains all units that are shipped with the SimBiology product. You can specify units for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the built-in units either by using the command sbiowhos -builtin -unit, or by accessing the root object.
- UnitPrefixes Contains all unit prefixes that are shipped with the SimBiology product. You can specify unit prefixes in combination with a valid unit for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the built-in unit prefixes either by using the command sbiowhos -builtin -unitprefix, or by accessing the root object.
- KineticLaws Contains all abstract kinetic laws that are shipped with the SimBiology product. Use the command sbiowhos -builtin -kineticlaw to see the list of built-in kinetic laws. You can use built-in kinetic laws when you use the command addkineticlaw to create a kinetic law object for a reaction object. Refer to the kinetic law by name when you create the kinetic law object, for example, kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');.

See "Abstract Kinetic Law" on page 6-49 for a definition and more information.

#### Characteristics BuiltInLibrary

Applies to	Object: root
Data type	object
Data values	Unit, unit prefix, and abstract kinetic law objects
Access	Read-only

Characteristics for BuiltInLibrary properties:

• Units

Applies to Data type Data values Access BuiltInLibrary property unit objects units Read-only

- UnitPrefixes
  - Applies to Data type Data values Access

BuiltInLibrary property Unit prefix objects Uunit prefixes Read-only

• KineticLaws

Applies to Data type Data values Access BuiltInLibrary property Abstract kinetic law object Kinetic laws Read-only

#### Examples I

#### **Example 1**

This example uses the command sbiowhos to show the current list of built-in components.

```
sbiowhos -builtin -kineticlaw
sbiowhos -builtin -unit
sbiowhos -builtin -unitprefix
```

#### Example 2

This example shows the current list of built-in components by accessing the root object.

```
rootObj = sbioroot;
get(rootObj.BuiltinLibrary, 'KineticLaws')
get(rootObj.BuiltinLibrary, 'Units')
get(rootObj.BuiltinLibrary, 'UnitPrefixes')
```

```
See Also sbioaddtolibrary, sbioremovefromlibrary sbioroot, sbiounit, sbiounitprefix, UserDefinedLibrary
```

## **BuiltInUnitPrefixes**

Purpose	Contain built-in unit prefixes	
	<b>Note</b> BuiltInUnitPrefixes h Use BuiltInLibrary instead.	as been removed and produces an error.
Description	BuiltInUnitPrefixes is a SimBiology root object property showing all unit prefixes that are shipped with SimBiology. You can specify units with prefixes for species amounts and parameter values to do dimensional analysis and unit conversion during simulation. The valid units and unit prefixes are either built-in or user-defined. You can display the built-in unit prefixes either by using the command sbiowhos, or by accessing the root object.	
	You cannot add, modify, or dele	te BuiltInUnitsPrefixes.
Characteristics	Applies to	Object: root
	Data type	char string
	Data values	Valid units
	Access	Read-only
See Also	BuiltInLibrary	

Purpose	Contain built-in units		
	<b>Note</b> BuiltInUnits has been removed and produces an error. Use BuiltInLibrary instead.		
Description	BuiltInUnits is a SimBiology root object property showing all units that are shipped with SimBiology. You can specify units for species amounts and parameter values to do dimensional analysis and unit conversion during simulation. The valid units are either built-in or user-defined. You can display the built-in units either by using the command sbiowhos, or by accessing the root object.		
	You cannot add, modify, or delete BuiltInUnits.		
<b>Characteristics</b>			
	Applies to	Object: root	
	Data type	char string	
	Data values	Valid units	
	Access	Read-only	
See Also	BuiltInLibrary		

## Capacity

Purpose	Compartment capaci	ty	
Description	The Capacity property indicates the size of the SimBiology compartment object. If the size of the compartment does not vary during simulation set the property ConstantCapacity to true.		
	You can vary compar	rtment capacity using rules or events.	
	<b>Note</b> Remember to set the ConstantCapacity property to false for varying capacity.		
	Events cannot result in the capacity having a negative value. Rules could result in capacity having negative value.		
Characteristics	;		
	Applies to	Object: compartment	
	Data type	double	
	Data values	Positive real number. The default value is 1.	
	Access	Read/write	
Examples	Add a compartment t	to a model and set the capacity of the compartment.	
	1 Create a model object named my_model.		
	<pre>modelObj = sbiomodel ('comp_model');</pre>		
	L		
	<b>2</b> Add the compartment object with the name nucleus and a capacity of 0.5.		
	compartmentOb	j = addcompartment(modelObj, 'nucleus', 0.5);	
See Also	addcompartment, add	dspecies, CapacityUnits, ConstantCapacity	

#### Purpose Compartment capacity units

**Description** The CapacityUnits property indicates the unit definition for the Capacity property of a compartment object. CapacityUnits can be any unit from the units library. To get a list of the defined units in the library, use the sbioshowunits function. If CapacityUnits changes from one unit definition to another, the Capacity does not automatically convert to the new units. The sbioconvertunits function does this conversion. To add a user-defined unit to the list, see sbioaddtolibrary.

#### **Characteristics**

	Applies to	Object: compartment
	Data type	char string
	Data values	Units from library with dimensions of length, area, or volume. Default = ' ' (empty).
	Access	Read/write
Example	1 Create a model obj	ect named my_model.
	modelObj = sb	iomodel ('my_model');
	<b>2</b> Add a compartment of 0.5.	nt object with the name cytoplasm and a capacity
	compObj = add	compartment (modelObj, 'cytoplasm', 0.5);
	<b>3</b> Set the CapacityU	nits to femtoliter, and verify.
		'CapacityUnits', 'femtoliter'); 'CapacityUnits')
	MATLAB returns:	
	ans =	

## **CapacityUnits**

femtoliter

## See Also InitialAmount, sbioaddtolibrary, sbioconvertunits, sbioshowunits

#### **Purpose** Array of compartments in model or compartment

**Description** Compartments shows you a read-only array of SimBiology compartment objects in the model object and the compartment object. In the model object, the Compartments property indicates all the compartments in a Model object as a flat list. In the compartment object, the Compartments property indicates other compartments that are referenced within the compartment. The two instances of Compartments are illustrated in "Examples" on page 6-19.

You can add a compartment object using the method addcompartment.

#### **Characteristics**

Applies to	Objects: compartment, model
Data type	Array of compartment objects
Data values	Compartment object. Default is [] (empty).
Access	Read-only

**Examples** 1 Create a model object named modelObj.

modelObj = sbiomodel('cell');

**2** Add two compartments to the model object.

compartmentObj1 = addcompartment(modelObj, 'nucleus'); compartmentObj2 = addcompartment(modelObj, 'mitochondrion');

**3** Add a compartment to one of the compartment objects.

compartmentObj3 = addcompartment(compartmentObj2, 'matrix');

4 Display the Compartments property in the model object.

get(modelObj, 'Compartments')

SimBiology Compartment Array

Index:	Name:	Capacity:	CapacityUnits:
1	nucleus	1	
2	mitochondrion	1	
3	matrix	1	

**5** Display the Compartments property in the compartment object.

get(compartmentObj2, 'Compartments')
SimBiology Compartment - matrix
Compartment Components:
 Capacity: 1
 CapacityUnits:
 Compartments: 0
 ConstantCapacity: true
 Owner: mitochondrion
 Species: 0

See Also addcompartment, addreaction, addspecies, Compartment object

#### **Purpose** Dimensional analysis and unit conversion options

**Description** The SimBiology CompileOptions property is an object that defines the compile options available for simulation; you can specify whether dimensional analysis and unit conversion is necessary for simulation. Compile options are checked during compile time. The compile options object can be accessed through the CompileOptions property of the configset object. Retrieve CompileOptions object properties with the get function and configure the properties with the set function.

DefaultSpeciesDimension	Species dimension
DimensionalAnalysis	Perform dimensional analysis on model
Туре	Display top-level SimBiology object type
UnitConversion	Perform unit conversion
	DimensionalAnalysis Type

#### **Characteristics**

Applies to	Object: configset
Data type	Object
Data values	Compile-time options
Access	Read-only

**Example** 1 Retrieve the configset object of modelObj.

modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj);

2 Retrieve the CompileOptions object (optionsObj) from the configsetObj.

optionsObj = get(configsetObj, 'CompileOptions');

Compile Settings:

UnitConversion:	false
DimensionalAnalysis:	true

See Also

get, set

#### Purpose Unit composition

**Description** The Composition property holds the composition of a unit object. The Composition property shows the combination of base and derived units that defines the unit. For example, molarity is the name of the unit and the composition is mole/liter. Base units are the set of units used to define all unit quantity equations. Derived units are defined using base units or mixtures of base and derived units.

Valid physical quantities for reaction rates are amount/time, mass/time, or concentration/time.

#### **Characteristics**

Applies to	Object: Unit
Data type	char string
Data values	Valid combination of units and prefixes from the library. Default is ' ' (empty).
Access	Read/write

## **Examples** This example shows you how to create a user-defined unit, add it to the user-defined library, and query the Composition property.

1 Create a unit for the rate constants of a second-order reaction.

unitObj = sbiounit('secondconstant', '1/molarity\*second', 1);

2 Query the Composition property.

```
get(unitObj, 'Composition')
ans =
1/molarity*second
```

**3** Change the Composition property.

```
set(unitObj, 'Composition', 'liter/mole*second'))
ans =
liter/mole*second
4 Add the unit to the user-defined library.
sbioaddtolibrary(unitObj);
See Also
get, Multiplier, Offset, sbiounit, set
```

#### **Purpose** Specify variable or constant species amount

#### Description

The ConstantAmount property indicates whether the quantity of the species object can vary during the simulation. ConstantAmount can be either true or false. If ConstantAmount is true, the quantity of the species cannot vary during the simulation. By default, ConstantAmount is false and the quantity of the species can vary during the simulation. If ConstantAmount is false, the quantity of the species can be determined by reactions and rules.

The property ConstantAmount is for species objects; the property ConstantValue is for parameter objects.

#### **More Information**

The following is an example of modeling species as constant amounts:

Modeling the role of nucleotides (GTP, ATP, cAMP) and cofactors (Ca<sup>++</sup>, NAD<sup>+</sup>, coenzyme A). Consider the role of GTP in the activation of Ras by receptor tyrosine kinases.

Ras-GDP + GTP -> Ras-GTP + GDP

Model GTP and GDP with constant amount set to true. In addition, you can set the BoundaryCondition of these species to true, thus making them *boundary species*.

#### **Characteristics**

	Applies to	Object: species	
	Data type	boolean	
	Data values	true or false. The default value is false.	
	Access	Read/write	
Examples	<pre>1 Create a model object named my_model.</pre>		
	modelObj = sbiomodel ('my_model');		

#### **Purpose** Specify variable or constant compartment capacity

**Description** The ConstantCapacity property indicates whether the capacity of the compartment object can vary during the simulation. ConstantCapacity can be either true (1) or false (0). If ConstantCapacity is true, the quantity of the compartment cannot vary during the simulation. By default, ConstantCapacity is true and the quantity of the compartment cannot vary during the simulation. If ConstantCapacity is false, the quantity of the compartment can be determined by rules and events.

#### **Characteristics**

Applies to	Object: compartment
Data type	boolean
Data values	true or false. The default value is true.
Access	Read/write

- **Examples** Add a compartment to a model and check the ConstantCapacity property of the compartment.
  - **1** Create a model object named comp\_model.

modelObj = sbiomodel ('comp\_model');

**2** Add the compartment object with the name nucleus and with a capacity of 0.5.

compartmentObj = addcompartment(modelObj, 'nucleus', 0.5);

**3** Display the ConstantCapacity property.

```
get(compartmentObj, 'ConstantCapacity')
```

ans =

1

See Also addcompartment, ConstantAmount, ConstantValue

#### **Purpose** Specify variable or constant parameter value

**Description** The ConstantValue property indicates whether the value of a parameter can change during a simulation. Enter either true (value is constant) or false (value can change).

You can allow the value of the parameter to change during a simulation by specifying a rule that changes the Value property of the parameter object.

The property ConstantValue is for parameter objects; the property ConstantAmount is for species objects.

#### **More Information**

As an example, consider feedback inhibition of an enzyme such as aspartate kinase by threonine. Aspartate kinase has three isozymes that are independently inhibited by the products of downstream reactions (threonine, homoserine, and lysine). Although threonine is made through a series of reactions in the synthesis pathway, for illustration, the reactions are simplified as follows:

Aspartic acid  $\xrightarrow{\text{aspartate kinase}} \beta - Aspartylphosphate$ 

 $\beta$ -Aspartylphosphate  $\longrightarrow$  Threonine

To model inhibition of aspartate kinase by threonine, you could use a rule like the algebraic rule below to vary the rate of the above reaction and simulate inhibition. In the rule, the rate constant for the above reaction is denoted by k\_aspartate\_kinase and the quantity of threonine is threonine.

k\_aspartate\_kinase -(1/threonine)

#### **Characteristics**

Applies to	Object: parameter
Data type	boolean

# **ConstantValue**

	Data values	true or false. The default value is 'true'.
	Access	Read/write
Examples	<ol> <li>Create a model obj modelObj = sb</li> <li>Add a parameter o</li> </ol>	iomodel ('my_model');
	parameterObj	= addparameter (modelObj, 'kf');
	<b>3</b> Change the Consta default (true) to fa	antValue property of the parameter object from alse and verify.
	MATLAB returns	1 for true and 0 for false.
		rObj, 'ConstantValue', false); Obj, 'ConstantValue')
	MATLAB returns:	
	ans =	
	0	
See Also	addparameter	

#### **Purpose** Contents of variant object

**Description** The Content property contains the data for the variant object. Content is a cell array with the structure {'Type', 'Name', 'PropertyName', 'PropertyValue'}. You can store values for species InitialAmount, parameter Value, and compartment Capacity, in a variant object.

For more information about variants, see Variant object.

#### **Characteristics**

Applies to	Object: variant
Data type	cell array
Data values	Default value is [](empty).
Access	Read/write

**Examples** 1 Create a model containing three species in one compartment.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
A = addspecies(compObj, 'A');
B = addspecies(compObj, 'B');
C = addspecies(compObj, 'C');
```

**2** Add a variant object that varies the species' InitialAmount property.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {{'species','A', 'InitialAmount', 5}, ...
{'species', 'B', 'InitialAmount', 10}});
% Display the variant
variantObj
```

SimBiology Variant - v1 (inactive)

ContentIndex:	Type:	Name:	Property:	Value:
1	species	A	InitialAmount	5
2	species	В	InitialAmount	10

**3** Append data to the **Content** property.

addcontent(variantObj, {'species', 'C', 'InitialAmount', 15});					
SimBiology Variant - v1 (inactive)					
	ContentIndex:	Type:	Name:	Property:	Value:
	1	species	А	InitialAmount	5
	2	species	В	InitialAmount	10
	3	species	C	InitialAmount	15
<pre>4 Remove a species from the Content property.     rmcontent(variantObj, 3);</pre>					
<b>5</b> Replace the data in the <b>Content</b> property.					
<pre>set(variantObj, 'Content', {'species', 'C', 'InitialAmount', 15});</pre>			ount', 15});		
See Also	addcontent, rmconten	t, sbiovari	lant		

#### Purpose Store simulation data

# **Description** The Data property contains the simulation data stored in the SimData object.

This property contains all data logged during a simulation, including species amounts, parameter values, and sensitivities. The property is an  $m \times n$  array, where m is the number of time steps in the simulation and n is the number of quantities logged. The rows of the array are labeled by the time points in the Time property, and the columns are labeled by the metadata in the DataInfo property.

#### **Characteristics**

Applies to	Object: SimData
Data type	double
Data values	Default value is [] (empty).
Access	Read-only

See Also DataInfo, ModelName

# DataCount

Purpose	Numbers of species, parameters, sensitivities		
Description	The DataCount property shows how many species, parameters, and sensitivities are logged in a SimData object. It is a MATLAB structure with the fields Species, Parameter, and Sensitivity. The information in this property is redundant with the DataInfo property and is there to give you a convenient means to access the information.		
Characteristics	i		
	Applies to	Object: SimData	
	Data type struct		
	Data values	Default value for each field is 0.	
	Access	Read-only	
See Also	StopTime, StopTimeType		

#### Purpose Metadata labels for simulation data

**Description** The DataInfo property contains the metadata that label the columns of the SimData object array. It is an n x 1 cell array of structures. The ith cell contains metadata labeling the ith column of the SimData object array.

The possible types of structures are as follows.

Туре	Fields
Species	Type: species Name: Compartment: Units:

# DataInfo

Туре	Fields
Parameter	Type: parameter Name: Reaction: <name a="" is="" of="" parameter="" reaction="" scoped="" that="" to,<br="">or '' if parameter is scoped to model&gt; Units:</name>
Sensitivity	Type: sensitivity Name: <for d[x]="" d[y]_0="" example:=""> OutputType: <the of="" output,<br="" sensitivity="" the="" type="">either 'species' or 'parameter'&gt; OutputName: <the name="" of="" output="" sensitivity="" the=""> OutputQualifier: <the compartment="" for<br="" or="" reaction="">the sensitivity output, for species or parameters, respectively&gt; InputType: <the input,<br="" of="" sensitivity="" the="" type="">either 'species' or 'parameter'&gt; InputName: <the input="" name="" of="" sensitivity="" the=""> InputQualifier: <the compartment="" for<br="" or="" reaction="">the sensitivity input, for species or parameters, respectively&gt; Units:</the></the></the></the></the></the></for>

## **Characteristics**

Applies to	Object: SimData
Data type	n x 1 cell array of structs
Data values	Default value is 0x1 cell array.
Access	Read-only

See Also

StopTime, StopTimeType

Purpose	Show names	s in SimData object
---------	------------	---------------------

**Description** The DataNames property holds the names that label the columns of the data matrix in the Data property. The property contains an nx1 array of strings. The software provides this information for your convenience.

#### **Characteristics**

Applies to	Object: SimData
Data type	string array
Data values	Default value is 0x1 cell array.
Access	Read-only

See Also StopTime, StopTimeType

# **DefaultSpeciesDimension**

Purpose	Species dimension	
Description	The DefaultSpeciesDimension property specifies whether the species dimensions are substance or concentration. If however, you specify the species units in the InitialAmountUnits property, these units define the species dimension regardless of the value in DefaultSpeciesDimension. Thus, if DefaultSpeciesDimension is concentration and you specify species units as molecule, the species dimensions are evaluated as substance.	
	You can find DefaultSpeciesDimension in the CompileOptions property.	
	When DefaultSpeciesDimension is set to substance, species quantities ignore compartment capacity, unless capacity is explicitly defined in an expression (reaction rate, rule, or event expression).	
	When DefaultSpeciesDimension is set to concentration, species quantities are scaled for compartment capacity in reaction rate, rule, or event expressions. CompartmentCapacity has a default value of 1, thus when capacity and capacity unit are not defined, species amount is equivalent to concentration.	
	For example, consider a reaction $a + b > c$ . Using mass action kinetics, the reaction rate is defined as $a*b*k$ , where k is the rate constant of the reaction. If you specify that initial amounts of a and b are 0.01M and 0.005M respectively, then units of k are 1/(M*second). If you specify k with another equivalent unit definition, for example, 1/[(moles/liter)*second], DimensionalAnalysis checks whether the physical quantities match. If the physical quantities do not match, you see an error and the model is not simulated.	
	If in the above example, you define initial amounts of a and b are 0.01 and 0.005 respectively, without specifying units, the compile options check whether DefaultSpeciesDimension is substance or concentration. If the DefaultSpeciesDimension is concentration, and the reaction rate dimensions resolve to concentration/time the model is simulated with species amounts scaled for compartment capacity, and the solver returns the species values in concentration.	

Valid physical quantities for reaction rates are amount/time, mass/time, or concentration/time.

#### **Characteristics**

Applies to	Object: CompileOptions (in configset object)
Data type	char string
Data values	concentration or substance. Default value is concentration.
Access	Read/write

See Also CompileOptions, DimensionalAnalysis, get, getconfigset, sbiosimulate, set

# **DimensionalAnalysis**

#### **Purpose** Perform dimensional analysis on model

# **Description** The DimensionalAnalysis property specifies whether to perform dimensional analysis on the model before simulation. It is a property of the CompileOptions object. CompileOptions holds the model's compile time options and is the object property of the configset object. When DimensionalAnalysis is set to true, the SimBiology software checks whether the physical quantities of the units involved in reactions and rules, match and are applicable.

For example, consider a reaction a + b > c. Using mass action kinetics, the reaction rate is defined as a\*b\*k, where k is the rate constant of the reaction. If you specify that initial amounts of a and b are 0.01M and 0.005M respectively, then units of k are 1/(M\*second). If you specify k with another equivalent unit definition, for example, 1/[(moles/liter)\*second], DimensionalAnalysis checks whether the physical quantities match. If the physical quantities do not match, you see an error and the model is not simulated.

Unit conversion requires dimensional analysis. If DimensionalAnalysis is off, and you turn UnitConversion on, then DimensionalAnalysis is turned on automatically. If UnitConversion is on and you turn off DimensionalAnalysis, then UnitConversion is turned off automatically.

If you have MATLAB function calls in your model, dimensional analysis ignores any expressions containing function calls and generates a warning.

Valid physical quantities for reaction rates are amount/time, mass/time, or concentration/time.

#### **Characteristics**

Applies to	Object: CompileOptions (in configset object)
Data type	boolean

	Data values	true or false. Default value is true.
	Access	Read/write
Examples	-	ow to retrieve and set DimensionalAnalysis to false in the default configuration set in a
	1 Import a model.	
	modelObj = sbml	limport('oscillator')
	SimBiology Mode	el - Oscillator
	Model Compor	nents:
	Models:	0
	Parameters	
	Reactions	42
	Rules:	0
	Species:	23
	<b>2</b> Retrieve the config	set object of the model object.
	configsetObj =	getconfigset(modelObj)
	-	Settings - default (active) e: ode15s
	SolverType StopTime:	10.00000
	SolverOption	
	AbsoluteTo RelativeTo	
	RuntimeOptic StatesToLc	

CompileOptions: UnitConversion: true DimensionalAnalysis: true 3 Retrieve the CompileOptions object. optionsObj = get(configsetObj, 'CompileOptions') Compile Settings: UnitConversion: true DimensionalAnalysis: true 4 Assign a value of false to DimensionalAnalysis. set(optionsObj, 'DimensionalAnalysis', false) See Also get, getconfigset, sbiosimulate, set

#### **Purpose** Specify explicit or implicit tau error tolerance

**Description** The ErrorTolerance property specifies the error tolerance for the explicit tau and implicit tau stochastic solvers. It is a property of the SolverOptions object. SolverOptions is a property of the configset object. The explicit and implicit tau solvers automatically chooses a time interval (tau) such that the relative change in the propensity function for each reaction is less than the user-specified error tolerance.

A propensity function describes the probability that the reaction will occur in the next smallest time interval, given the conditions and constraints.

If the error tolerance is too large, there may not be a solution to the problem and that could lead to an error. If the error tolerance is small, the solver will take more steps than when the error tolerance is large leading to longer simulation times. The error tolerance should be adjusted depending upon the problem, but a good value for the error tolerance is between 1 % to 5 %.

#### **Characteristics**

Applies to	Object: SolverOptions
Data type	double
Data values	>0, <1. The default is $3e-2$ .
Access	Read/write

**Examples** This example shows how to change ErrorTolerance settings.

 Retrieve the configset object from the modelObj and change the SolverType to expltau.

modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj); set(configsetObj, 'SolverType', 'expltau')

**2** Change the ErrorTolerance to 1e-8.

set(configsetObj.SolverOptions, 'ErrorTolerance', 5.0e-2); get(configsetObj.SolverOptions, 'ErrorTolerance') ans = 5.000000e-002

See Also LogDecimation, RandomState

## **EventFcns**

#### Purpose Event expression

# **Description** Property of the event object that defines what occurs when the event is triggered. Specify a cell array of strings.

EventFcns can be any MATLAB assignment or expression that defines what is executed when the event is triggered. All EventFcn expressions are assignments of the form 'objectname = expression', where objectname is the name of a valid SimBiology object.

For more information about how SimBiology handles events, see "How Events Are Evaluated" in the SimBiology User's Guide documentation. For examples of event functions, see "Specifying Event Functions" in the SimBiology User's Guide documentation.

#### **Characteristics**

	Applies to	Object: event	
	Data type	Cell array of strings	
	Data values	EventFcn strings '' (empty)	
	Access	Read/write	
Examples	1 Create a model obje	ect, and then add an event object.	
	<pre>modelObj = sbmlimport('oscillator'); eventObj = addevent(modelObj, 'time&gt;= 5', 'OpC = 200');</pre>		
	<b>2</b> Set the EventFcns property of the event object.		
	<pre>set(eventObj, 'EventFcns', {'pA = OpA',</pre>	<pre>'EventFcns', {'pA = OpA','mA = pol'});</pre>	
	$\textbf{3} \; \mathrm{Get} \; \mathrm{the} \; \mathtt{EventFcns}$	property.	
	get(eventObj,	'EventFcns')	
See Also	Event object, Trigge	er	

## **Events**

Purpose	Contain all event objects	
Description	Property to indicate events in a model object. Read-only array of Event objects.	
	An event defines an action when a defined condition is met. For example, the quantity of a species may double when the quantity of species B is 100. An event is triggered when the conditions specified in the event are met by the model. See "Changing Model Component Values Using Events" in the SimBiology User's Guide documentation for more information.	
	Add an event to a Model object with the method addevent method and remove an event with the delete method. See Event object for more information.	
	You can view event object properties with the get command and modify the properties with the set command.	
Characteristics		
	Applies to	Object: model
	Data type	Array of event objects
	Data values	Event object. The default is [] (empty).
	Access	Read-only
Examples	1 Create a model object, and then a	add an event object.
	<pre>modelObj = sbmlimport('oscillator') eventObj = addevent(modelObj, 'time&gt;= 5', 'OpC = 200');</pre>	
	<b>2</b> Get a list of properties for an event object.	
	<pre>get(modelObj.Events(1));</pre>	
	Or	

get(eventObj)

MATLAB displays a list of event properties.

```
Active: 1

Annotation: ''

EventFcns: {'OpC = 200'}

Name: ''

Notes: ''

Parent: [1x1 SimBiology.Model]

Tag: ''

Trigger: 'time >= 5'

TriggerDelay: 0

TriggerDelayUnits: 'second'

Type: 'event'

UserData: []
```

See Also EventFcns, Event object, Model object, Trigger

# Exponent

Purpose	Exponent value of unit prefix	
Description	<i>Exponent</i> shows the value of 10 <sup>Exponent</sup> that defines the numerical value of the unit prefix <i>Name</i> . You can use the unit prefix in conjunction with any built-in or user-defined units. For example, for the unit mole, specify as picomole to use the Exponent, -12.	
Characteristics	Applies to Data type Data values	Object: Unit prefix double Real number. Default is 0.
	Access	Read/write
Examples	<pre>This example shows you how to create a user-defined unit prefix, add it to the user-defined library, and query the Exponent property. 1 Create a unit prefix.     unitprefixObj1 = sbiounitprefix('peta', 15); 2 Add the unit prefix to the user-defined library.     sbioaddtolibrary(unitprefixObj1); 3 Query the Exponent property.</pre>	
	<pre>get(unitprefixObj1, 'Exponent')</pre>	
	ans =	
	15	
See Also	get, sbioaddtolibrary	, sbiounitprefix, set, UnitPrefix object

#### **Purpose** Expression to determine reaction rate equation

#### **Description**

The Expression property indicates the mathematical expression that is used to determine the ReactionRate property of the reaction object. Expression is a reaction rate expression assigned by the abstract kinetic law used by the kinetic law object. The abstract kinetic law being used is indicated by the property KineticLawName. You can configure Expression for user-defined abstract kinetic laws, but not for built-in abstract kinetic laws. Expression is read only for kinetic law objects.

#### **Abstract Kinetic Law**

The *abstract kinetic law* provides a mechanism for applying a specific rate law to multiple reactions. It acts as a mapping template for the reaction rate. The abstract kinetic law is defined by a reaction rate expression, which is defined in the property Expression, and the species and parameter variables used in the expression. The species variables are defined in the SpeciesVariables property, and the parameter variables are defined in the ParameterVariablesproperty of the kinetic law object.

If a reaction is using an abstract kinetic law, the ReactionRate property of the reaction object shows the result of a mapping from an abstract kinetic law. To determine ReactionRate, the species variables and parameter variables that participate in the reaction rate should be clearly mapped in the kinetic law for the reaction. In this case, SimBiology software determines the ReactionRate by using the Expression property of the abstract kinetic law object, and by mapping SpeciesVariableNames to SpeciesVariables and ParameterVariableNames to ParameterVariables.

For example, the abstract kinetic law Henri-Michaelis-Menten has the Expression, Vm\*S/(Km+S), where Vm and Km are defined as parameters in the ParameterVariables property of the abstract kinetic law object, and S is defined as a species in the SpeciesVariable property of the abstract kinetic law object.

By applying the abstract kinetic law Henri-Michaelis-Menten to a reaction A -> B with Va mapping to Vm, A mapping to S, and Ka mapping to Km, the rate equation for the reaction becomes  $Va^*A/(Ka+A)$ .

The exact expression of a reaction using MassAction kinetic law varies depending upon the number of reactants. Thus, for mass action kinetics the Expression property is set to MassAction because in general for mass action kinetics the reaction rate is defined as

$$r = k \prod_{i=1}^{n_r} [Si]^{m_i}$$

where [Si] is the concentration of the ith reactant,  $m_i$  is the stoichiometric coefficient of [Si],  $n_r$  is the number of reactants, and k is the mass action reaction rate constant.

SimBiology software comes with some built-in kinetic laws. Users can also define their own abstract kinetic laws. To find the list of available kinetic laws, use the sbiowhos -kineticlaw command (sbiowhos). You can create an abstract kinetic law with the function sbioabstractkineticlaw and add it to the library using sbioaddtolibrary.

#### **Characteristics**

Applies to	Objects: abstract kineticlaw, kineticlaw
Data type	char string
Data values	Defined by abstract kinetic law
Access	Read-only in kinetic law object. Read/write in user-defined abstract kinetic law.

#### Examples

#### Example 1

Example with Henri-Michaelis-Menten kinetics

1 Create a model object, and add a reaction object to the model.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2 Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

**3** Verify that the Expression property for the kinetic law object is Henri-Michaelis-Menten.

get (kineticlawObj, 'Expression')

MATLAB returns:

ans = Vm\*S/(Km + S)

4 The 'Henri-Michaelis-Menten' kinetic law has two parameter variables (Vm and Km) and one species variable (S) that you should set. To set these variables, first create the parameter variables as parameter objects (parameterObj1, parameterObj2) with names Vm\_d, Km\_d, and assign the objects' Parent property value to the kineticlawObj. The species object with Name a is created when reactionObjis created and need not be redefined.

```
parameterObj1 = addparameter(kineticlawObj, 'Vm_d');
parameterObj2 = addparameter(kineticlawObj, 'Km d');
```

5 Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Vm_d' 'Km_d'});
set(kineticlawObj,'SpeciesVariableNames', {'a'});
```

**6** Verify that the reaction rate is expressed correctly in the reaction object ReactionRate property.

```
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

ans =

Vm d\*a/(Km d+a)

#### **Example 2**

Example with Mass Action kinetics.

1 Create a model object, and then add a reaction object.

modelObj = sbiomodel ('my\_model'); reactionObj = addreaction (modelObj, 'a + b -> c + d');

**2** Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
get(kineticlawObj, 'Expression')
```

MATLAB returns:

ans =

MassAction

**3** Assign the rate constant for the reaction.

```
set (kineticlawObj, 'ParameterVariablenames', 'k');
```

get (reactionObj, 'ReactionRate')

MATLAB returns:

ans =

k\*a\*b

See Also KineticLawName, Parameters, ParameterVariableNames, ParameterVariables, ReactionRate, sbioaddtolibrary, sbiowhos, SpeciesVariableNames, SpeciesVariables

# InitialAmount

Purpose	Species initial amount	
Description	The InitialAmount property indicates the initial quantity of the SimBiology species object. InitialAmount is the quantity of the species before the simulation starts.	
Characteristics		
	Applies to	Object: species
	Data type	double
	Data values	Positive real number. Default value is 0.
	Access	Read/write
Examples	Add a species to a mo	del and set the initial amount of the species.
	Create a model object named my_model.	
	<pre>modelObj = sbiomodel ('my_model');</pre>	
	<b>2</b> Add the species object named glucose.	
	<pre>speciesObj = addspecies (modelObj, 'glucose');</pre>	
	<b>3</b> Set the initial amo	unt to 100 and verify.
	set (speciesObj, 'InitialAmount',100); get (speciesObj, 'InitialAmount')	
	MATLAB returns:	
	ans =	
	100	
See Also	addspecies, Initial	AmountUnits

#### **Purpose** Species initial amount units

# **Description** The InitialAmountUnits property indicates the unit definition for the InitialAmount property of a species object. InitialAmountUnits can be one of the built-in units. To get a list of the defined units, use the sbioshowunits function. If InitialAmountUnits changes from one unit definition to another, InitialAmount does not automatically convert to the new units. The sbioconvertunits function does this conversion. To add a user-defined unit to the list, see sbioregisterunit.

See DefaultSpeciesDimension for more information on specifying dimensions for species quantities. InitialAmountUnits must have corresponding dimensions to CapacityUnits. For example, if the CapacityUnits are meter<sup>2</sup>, then species must be amount/meter<sup>2</sup> or amount.

#### **Characteristics**

	Applies to	Object: species	
	Data type	char string	
	Data values	Units from library with dimensions of amount, amount/length, amount/area, or amount/volume. Default is '' (empty).	
	Access	Read/write	
Examples	modelObj = sb	ject named my_model. iomodel ('my_model'); compartment(modelObj, 'cell');	
	<b>2</b> Add a species obje	ct named glucose.	
	<pre>speciesObj = addspecies (compObj, 'glucose');</pre>		
	<b>3</b> Set the initial amo and verify.	ount to 100, InitialAmountUnits to molecule,	

set (speciesObj,'InitialAmountUnits','molecule');
get (speciesObj,'InitialAmountUnits')
MATLAB returns:
 ans =
 molecule
DefaultSpeciesDimension\_InitialAmount\_sbioconvertunits

See Also DefaultSpeciesDimension, InitialAmount, sbioconvertunits, sbioregisterunit, sbioshowunits

#### **Purpose** Show kinetic law used for ReactionRate

# **Description** The KineticLaw property shows the kinetic law that determines the reaction rate specified in the ReactionRate property of the reaction object. This property shows the kinetic law used to define ReactionRate.

KineticLaw can be configured with the addkineticlaw method. The addkineticlaw function configures the ReactionRate based on the KineticLaw and the species and parameters specified in the kinetic law object properties SpeciesVariableNames and ParameterVariableNames. SpeciesVariableNames are determined automatically for mass action kinetics.

If the reaction is updated, the ReactionRate is automatically updated only for mass action kinetics. For all other kinetics, the SpeciesVariableNames property of the kinetic law object should be reconfigured.

#### **Characteristics**

Applies to	Object: reaction
Data type	Kinetic law object
Data values	Kinetic law object. Default is [] (empty).
Access	Read-only

#### **Example** Example with Henri-Michaelis-Menten kinetics

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

2 Define a kinetic law for the reaction object.

kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');

# **KineticLaw**

	<b>3</b> Verify that the KineticLaw property for the reaction object is Henri-Michaelis-Menten.			
	get (reactionObj, 'KineticLaw')			
	MATLAB returns:			
	SimBiology Kinetic Law Array			
	Index: KineticLawName: 1 Henri-Michaelis-Menten			
See Also	KineticLawName, Parameters, ParameterVariableNames, ReactionRate, SpeciesVariableNames			

#### **Purpose** Name of kinetic law applied to reaction

**Description** The KineticLawName property of the kinetic law object indicates the name of the abstract kinetic law applied to the reaction. KineticLawName can be any valid name from the built-in or user-defined abstract kinetic law library. See "Abstract Kinetic Law" on page 6-49 for a definition and more information.

> You can find the KineticLawName list in the abstract kinetic law library by using the command sbiowhos -kineticlaw (sbiowhos). You can create an abstract kinetic law with the function sbioabstractkineticlaw and add it to the library using sbioaddtolibrary.

#### **Characteristics**

Applies to	Object: kineticlaw
Data type	char string
Data values	char string defined by abstract kinetic law
Access	Read-only

**Examples** 1 Create a model object, add a reaction object, and define a kinetic law for the reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

**2** Verify the KineticLawName of kineticlawObj.

```
get (kineticlawObj, 'KineticLawName')
```

MATLAB returns:

ans =

# **KineticLawName**

Henri-Michaelis-Menten

#### See Also

Expression, Parameters, ParameterVariableNames, ParameterVariables, ReactionRate, sbioaddtolibrary, sbiowhos, SpeciesVariables, SpeciesVariableNames

#### **Purpose** Specify recorded simulation output frequency

**Description** The LogDecimation property defines how often the simulation data is recorded as output. It is a property of the SolverOptions object. SolverOptions is a property of the configset object. LogDecimation is available for ssa, expltau, and inmpltau solvers.

Use LogDecimation to specify how frequently you want to record the output of the simulation. For example, if the LogDecimation is set to 1, for the command (t,x) = sbiosimulate(modelObj), at each simulation step the time will be logged in t and the quantity of each logged species will be logged as a row in x. If LogDecimation is 10, then every 10th simulation step will be logged in t and x.

#### **Characteristics**

Applies to	Object: SolverOptions
Data type	int
Data values	>0. Default is 1.
Access	Read/write

**Examples** This example shows how to change LogDecimation settings.

1 Retrieve the configset object from the modelObj, and change the SolverType to expltau.

modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj); set(configsetObj, 'SolverType', 'expltau')

2 Change the LogDecimation to 10.

```
set(configsetObj.SolverOptions, 'LogDecimation', 10);
get(configsetObj.SolverOptions, 'LogDecimation')
```

```
ans =
```

# LogDecimation

10

See Also ErrorTolerance, RandomState

#### **Purpose** Specify nonlinear solver maximum iterations in implicit tau

# **Description** The MaxIterations property specifies the maximum number of iterations for the nonlinear solver in impltau. It is a property of the SolverOptions object. SolverOptions is a property of the configset object.

The implicit tau solver in SimBiology software internally uses a nonlinear solver to solve a set of algebraic nonlinear equations at every simulation step. Starting with an initial guess at the solution, the nonlinear solver iteratively tries to find the solution to the algebraic equations. The closer the initial guess is to the solution, the fewer the iterations the nonlinear solver will take before it finds a solution. MaxIterations specifies the maximum number of iterations the nonlinear solver should take before it issues a "failed to converge" error. If you get this error, during simulation, try increasing MaxIterations. The default value of MaxIterations is 15.

#### **Characteristics**

Applies to	Object: SolverOptions
Data type	int
Data values	>0. Default is 15.
Access	Read/write

#### **Examples** This example shows how to change MaxIterations settings.

 Retrieve the configset object from the modelObj, and change the SolverType to impltau.

modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj); set(configsetObj, 'SolverType', 'impltau');

2 Change the MaxIterations to 25.

```
set(configsetObj.SolverOptions, 'MaxIterations', 25);
```

See Also

get(configsetObj.SolverOptions, 'MaxIterations') ans = 25 ErrorTolerance,LogDecimation,RandomState

#### **Purpose** Specify upper bound on solver step size

**Description** The MaxStep property specifies the size of the bounds on the size of the time steps. If the differential equation has periodic coefficients or solutions, it might be a good idea to set MaxStep to some fraction (such as 1/4) of the period. This guarantees that the solver does not enlarge the time step too much and step over a period of interest. For more information on MaxStep, see odeset in the MATLAB documentation.

#### **Characteristics**

See Also

Applies to	Object: SolverOptions	
Data type	Positive scalar	
Data values	<pre>{0.1*abs(t0-tf)}. Default is [] (empty).</pre>	
Access	Read/write	
SimBiology property RelativeTolerance		

MATLAB function odeset

## ModelName

Purpose	Name of model simulated	
Description	The ModelName property shows the name of the model for which the SimData object contains the simulation data.	
<b>Characteristics</b>		
	Applies to	Object: SimData
	Data type	string
	Data values	Default value is '' (empty).
	Access	Read-only
See Also	Data, DataInfo	

Purpose	Contain all model objects		
	Submodels will not b	coperty will be removed in a future version. e supported in future releases. Use the function rt submodels into models.	
Description	The Models property shows the submodels in a model object or models in the SimBiology root. Read-only array of model objects. SimBiology has a hierarchical organization. A top-level model object has the SimBiology root as its Parent. Model objects with another model object as Parent are submodels. For a model object to access configset, kinetic law, reaction, rule and species objects, you must assign the model object as Parent in these objects. Parameter objects can have a model object or kinetic law object as Parent. You can display all the component objects with modelObj.Models or get (modelObj, 'Models').		
	The components of a submodel are contained within the submodel. In addition, a submodel object can reference parameter variables that have been assigned to the model object. For example, a parameter defined within a submodel cannot be used by the parent model or another model object. A submodel object however, can use the parameters assigned to the model object.		
	You can add a submodel to a model object with the method addmodel and remove it from its parent with the method delete.		
Characteristics	Applies to Data type Data values Access	Objects: model, root Array of model objects Model object. Default is [] (empty). Read-only	
See Also	sbiomodel, sbioupda	ate	

## **Multiplier**

Purpose	Relationship between defined unit and base unit	
Description	The Multiplier is the numerical value that defines the relationship between the unit Name and the base unit as a product of the Multiplier and the base unit. For example, in Celsius = (5/9)*( Fahrenheit-32); Multiplier is 5/9 and Offset is -32. For 1 mole = 6.0221e23*molecule, the Multiplier is 6.0221e23.	
Characteristics	Applies to Data type Data values Access	Object: Unit double Nonzero real number. Default value is 1. Read/write
Examples	<pre>Access Read/write This example shows how to create a user-defined unit, add it to the user-defined library, and query the library. 1 Create a user-defined unit called usermole, whose composition is molecule and Multiplier property is 6.0221e23.     unitObj = sbiounit('usermole', 'molecule', 6.0221e23); 2 Add the unit to the user-defined library.     sbioaddtolibrary(unitObj); 3 Query the Multiplier property.     get(unitObj, 'Multiplier')     ans =     1/molarity*second</pre>	
See Also	Composition, get, Offset, sbiounit, set	

#### Purpose Specify name of object

#### Description

The Name property identifies a SimBiology object. Compartments, species, parameters, and model objects can be referenced by other objects using the Name property, therefore Name must be unique for these objects. However, species names need only be unique within each compartment. Parameter names must be unique within a model (if at the model level), or within each kinetic law (if at the kinetic law level). This means that you can have nonunique species names if the species are in different compartments, and nonunique parameter names if the parameters are in different kinetic laws or at different levels. Note that having nonunique parameter names can cause the model to have shadowed parameters and that may not be best modeling practice. For more information on levels of parameters, see "Definition of Parameter Scope" in the SimBiology User's Guide documentation.

Use the function sbioselect to find an object with the same Name property value.

In addition, note the following constraints and reserved characters for the Name property in objects:

- Model names cannot be empty.
- Parameter names cannot be empty, or have the name time.
- If you have a parameter, a species, or compartment name that is not a valid MATLAB variable name, when you write an event function, an event trigger, a reaction, reaction rate equation, or a rule you must enclose that name in brackets. For example, enclose [DNA polymerase+] in brackets. In addition, if you have the same species in multiple compartments you must qualify the species with the compartment name, for example, nucleus.[DNA polymerase+], [nuclear complex].[DNA polymerase+].
- Species and compartment names cannot be empty, and note the following reserved words, characters, and constraints:

### Name

- The literal words null and time. Note that you can specify species names with these words contained within the name. For example, nullaminoacids or nullnucleotides.
- The characters ->, < >, [, and ].

For more information on valid MATLAB variable names, see genvarname and isvarname.

#### **Characteristics**

Characteristics			
	Applies to	Objects: abstract kinetic law, configuration set, compartment, event, kinetic law, model, parameter, reaction, rule, species, unit, or variant	
	Data type	char string	
	Data values	Any char string except reserved words and characters	
	Access	Read/write	
Example	<pre>I Create a model object named my_model. modelObj = sbiomodel ('my_model');</pre>		
	<b>2</b> Add a reaction object to the model object. Note the use of brackets because the names are not valid MATLAB variable names.		
	reactionObj = addreaction(modelObj, '[Aspartic acid] -> [beta-Aspartyl-PO4]') MATLAB returns: SimBiology Reaction Array		
		ction: partic acid] -> [beta-Aspartyl-PO4]	
	2 Sat the reaction No.	me and verify	

**3** Set the reaction Name and verify.

set (reactionObj, 'Name', 'Aspartate kinase reaction');
get (reactionObj, 'Name')
MATLAB returns:
 ans =
 Aspartate kinase reaction
See Also
 addcompartment, addkineticlaw, addmodel, addparameter,
 addreaction, addrule, addspecies, sbiomodel, sbiounit,

sbiounitprefix

## Normalization

Purpose	Specify normalization type for sensitivity analysis	sis

**Description** Normalization is a property of the SensitivityAnalysisOptions object. SensitivityAnalysisOptions is a property of the configuration set object. Use Normalization to specify the normalization for the computed sensitivities.

The following values let you specify the type of normalization. The examples show you how sensitivities of a species x with respect to a parameter k are calculated for each normalization type:

• 'None' specifies no normalization.

dx(t)dk

• 'Half' specifies normalization relative to the numerator (species quantity) only.

$$\left(\frac{1}{x(t)}\right)\left(\frac{dx(t)}{dk}\right)$$

• 'Full' specifies that the data should be made dimensionless.

$$\left(\frac{k}{x(t)}\right)\left(\frac{dx(t)}{dk}\right)$$

#### **Characteristics**

Applies to	Object: SensitivityAnalysisOptions
Data type	enum
Data values	'None', 'Half', 'Full'. Default is 'None'.
Access	Read/write

See Also ParameterInputFactors, SensitivityAnalysis, SensitivityAnalysisOptions, SpeciesInputFactors

**Description** Use the Notes property of an object to store comments about the object. You can include HTML tagging in the notes to render formatted text in the SimBiology desktop.

#### **Characteristics**

	Applies to	Objects: compartment, kinetic law, model, parameter, reaction, rule, species, unit, or unit prefix	
	Data type	char string	
	Data values	Any char string	
	Access	Read/write	
Example	<pre>I Create a model object. modelObj = sbiomodel ('my_model');</pre>		
	<b>2</b> Write notes for the model object.		
	set (modelObj	, 'notes', '09/01/05 experimental data')	
	<b>3</b> Verify the assignment.		
	get (modelObj, 'notes')		
	MATLAB returns:		
	ans =		
	09/01/05 expe	rimental data	
See Also	addkineticlaw, addmodel, addparameter, addreaction, addrule, addspecies, sbiomodel, sbiounit, sbiounitprefix		

## Offset

Purpose	Unit composition modifier		
Description	The Offset is the numerical value by which the unit composition is modified from the base unit. For example, Celsius = (5/9)*( Fahrenheit-32); Multiplier is 5/9 and Offset is -32.		
Characteristics	i		
	Applies to	Object: Unit	
	Data type	double	
	Data values	Real number. Default is 0.	
	Access	Read/write	
Examples	This example shows how to create a user-defined unit, add it to the user-defined library, and query the library.		
	Create a user-defined unit called celsius2, whose composition refers to fahrenheit, Multiplier property is 9/5, and Offset property is 32.		
	unitObj = sbiounit('celsius2','fahrenheit',9/5,32);		
	<b>2</b> Add the unit to the user-defined library.		
	<pre>sbioaddtolibrary(unit0bj);</pre>		
	<b>3</b> Query the Offset property.		
	get(unitObj, 'Offset')		
	ans =		
	32		
See Also	Composition, get, Mult sbiounit, set	iplier, sbioaddtolibrary, sbioshowunits,	

#### Purpose Owning compartment

**Description** Owner shows you the SimBiology compartment object that owns the compartment object. In the compartment object, the Owner property shows you whether the compartment resides within another compartment. The Compartments property indicates whether other compartments reside within the compartment. You can add a compartment object using the method addcompartment.

#### **Characteristics**

Applies to	Object: compartment
Data type	char string
Data values	Name of compartment object. Default is [].
Access	Read-only

#### **Examples** 1 Create a model object named modelObj.

modelObj = sbiomodel('cell');

2 Add two compartments to the model object.

compartmentObj1 = addcompartment(modelObj, 'nucleus'); compartmentObj2 = addcompartment(modelObj, 'mitochondrion');

**3** Add a compartment to one of the compartment objects.

compartmentObj3 = addcompartment(compartmentObj2, 'matrix');

4 Display the Owner property in the compartment objects.

```
get(compartmentObj3, 'Owner')
```

The result shows you the owning compartment and its components:

SimBiology Compartment - mitochondrion

```
Compartment Components:
Capacity: 1
CapacityUnits:
Compartments: 1
ConstantCapacity: true
Owner:
Species: 0
```

**5** Change the owning compartment.

set(compartmentObj3, 'Owner', compartmentObj1)

See Also Compartments, Parent

#### **Purpose** Specify parameter input factors for sensitivity analysis

**Description** ParameterInputFactors is a property of the SensitivityAnalysisOptions object. SensitivityAnalysisOptions is a property of the configuration set object. Use ParameterInputFactors to specify the parameters with respect to which you want to compute the sensitivities of the species states in your model. When you simulate a model with SensitivityAnalysis enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species specified in StatesToLog. For a description of the output, see the SensitivityAnalysisOptions property description.

#### **Characteristics**

	Applies to	$\operatorname{Object:}$ SensitivityAnalysisOptions	
	Data type	Parameter object or array of parameter objects	
	Data values	Parameter object array. Default is [] (empty).	
	Access	Read/write	
Examples	This example shows how to set ParameterInputFactors for sensitivity analysis.		
	<ol> <li>Import the radio decay model from the SimBiology demos.</li> <li>modelObj = sbmlimport('radiodecay');</li> <li>Retrieve the configuration set object from modelObj.</li> </ol>		
	<pre>configsetObj = getconfigset(modelObj);</pre>		
	<b>3</b> Add a parameter to the ParameterInputFactors property and display. Use the sbioselect function to retrieve the parameter object from the model.		

set(configsetObj.SensitivityAnalysisOptions,'ParameterInputFactors', ... sbioselect(modelObj, 'Type', 'parameter', 'Name', 'c')); get (configsetObj.SensitivityAnalysisOptions, 'ParameterInputFactors')

SimBiology Parameter Array

Index: Name: Value: ValueUnits: 1 c 0.5 1/second

See Also sbioselect, SensitivityAnalysis, SensitivityAnalysisOptions, SpeciesInputFactors

#### **Purpose** Array of parameter objects

#### **Description** The Parameters property indicates the parameters in a Model or KineticLaw object. Read-only array of Parameter objects. Display with modelObj.Parameters or get(modelObj, 'Parameters').

The scope of a parameter object is hierarchical and is defined by the parameter's parent. If a parameter is defined with a kinetic law object as its parent, then only the kinetic law object can use the parameter. If a parameter object is defined with a model object as its parent, then components such as rules, events, and kinetic laws (reaction rate equations) can use the parameter.

You can add a parameter to a model object, or kinetic law object with the method addparameter and delete it with the method delete.

You can view parameter object properties with the get command and configure properties with the set command.

#### **Characteristics**

Applies to	Objects: model, kineticlaw
Data type	Array of parameter objects
Data values	Parameter objects. Default value is [] (empty).
Access	Read-only

#### **Examples** 1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a + b -> c + d');
```

**2** Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

**3** Add a parameter and assign it to the kinetic law object (kineticlawObj);.

parameterObj1 = addparameter (kineticlawObj, 'K1'); get (kineticlawObj, 'Parameters') SimBiology Parameter Array Index: Name: Value: ValueUnits: 1 K1 1 **4** Add a parameter and assign it to the model object (modelObj); parameterObj1 = addparameter(modelObj, 'K2'); get(modelObj, 'Parameters') SimBiology Parameter Array Index: ValueUnits: Name: Value: 1 K2 1 See Also addparameter, delete, get, sbioparameter, set

#### **Purpose** Cell array of reaction rate parameters

# **Description** The ParameterVariableNames property shows the parameters used by the kinetic law object to determine the ReactionRate equation in the reaction object. Use setparameter to assign ParameterVariableNames. When you assign species to ParameterVariableNames, SimBiology software maps these parameter names to ParameterVariables in the kinetic law object.

If the reaction is using a kinetic law, the ReactionRate property of a reaction object shows the result of a mapping from an abstract kinetic law. The ReactionRate is determined by the kinetic law object Expression property by mapping ParameterVariableNames to ParameterVariables and SpeciesVariableNames to SpeciesVariables.

#### **Characteristics**

Applies to	Object: kineticlaw
Data type	Cell array of strings
Data values	Cell array of parameters
Access	Read/write

## **Examples** Create a model, add a reaction, and assign the SpeciesVariableNames for the reaction rate equation.

**1** Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

**2** Create a kinetic law object for the reaction object of type 'Henri-Michaelis-Menten'.

```
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

reactionObj KineticLaw property is configured to kineticlawObj.

**3** The 'Henri-Michaelis-Menten' kinetic law has two parameter variables (Vm and Km) that should to be set. To set these variables:

```
setparameter(kineticlawObj,'Vm', 'Va');
setparameter(kineticlawObj,'Km', 'Ka');
```

**4** Verify that the parameter variables are correct.

```
get (kineticlawObj, 'ParameterVariableNames')
```

MATLAB returns:

```
ans =
```

```
'Va' 'Ka'
```

See Also Expression, ParameterVariables, ReactionRate, setparameter, SpeciesVariables, SpeciesVariableNames

#### **Purpose** Parameters in abstract kinetic law

**Description** The ParameterVariables property shows the parameter variables that are used in the Expression property of the abstract kinetic law object. Used to determine the ReactionRate equation in the reaction object. Use the MATLAB function set to assign ParameterVariables to an abstract kinetic law. For more information, see abstract kinetic law.

#### **Characteristics**

Applies to	Objects: abstract kinetic law, kineticlaw
Data type	Cell array of strings
Data values	Defined by abstract kinetic law
Access	Read/write in abstract kinetic law. Read-only in kinetic law.

## **Example** Create a model, add a reaction, and assign the SpeciesVariableNames for the reaction rate equation.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

**2** Create a kinetic law object for the reaction object of the type 'Henri-Michaelis-Menten'.

kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');

reactionObj KineticLaw property is configured to kineticlawObj.

**3** The 'Henri-Michaelis-Menten' kinetic law has two parameter variables. To set these variables:

get (kineticlawObj, 'ParameterVariables')

MATLAB returns:

ans =

'Vm' 'Km'

**See Also** Expression, ParameterVariableNames, ReactionRate, set, setparameter, SpeciesVariables, SpeciesVariableNames

#### Purpose Indicate parent object

# **Description** The Parent property indicates the parent object for a SimBiology object (read-only). The Parent property indicates accessibility of the object. The object is accessible to the Parent object and other objects within the Parent object. The value of Parent depends on the type of object and how it was created. All models always have the SimBiology root as the Parent.

#### **More Information**

The following table shows you the different objects and the possible Parent value.

Object	Parent	
abstract kinetic law	• [] (empty) until added to library	
	<ul> <li>root object upon addition to library</li> </ul>	
compartment	model object	
event	model object or [] (empty)	
kinetic law	reaction object	
model	root object	
parameter	model object, kinetic law object, or [] (empty)	
reaction	model object or [] (empty)	
rule	model object or [] (empty)	
species	compartment	

## Parent

Object	Parent
variant	model object or [] (empty)
unit and unit prefixes	• [] (empty) until added to library
	<ul> <li>root object upon addition to library</li> </ul>

#### **Characteristics**

Applies to	Objects: abstract kinetic law, compartment, event, kinetic law, model, parameter, reaction, rule, species, variant, unit, or unit prefix
Data type	Object
Data values	SimBiology component object or [] (empty)
Access	Read-only

See Also addkineticlaw, addmodel, addparameter, addreaction, sbiomodel

#### Purpose Array of reaction products

## **Description** The Products property contains an array of SimBiology.Species objects.

Products is a 1-by-n species object array that indicates the species that are changed by the reaction. If the Reaction property is modified to use a different species, the Products property is updated accordingly.

You can add product species to the reaction with addproduct function. You can remove product species from the reaction with rmproduct. You can also update reaction products by setting the Reaction property with the function set.

#### **Characteristics**

	Applies to	Object: reaction	
	Data type	Array of objects	
	Data values	Species objects. Default is [] (empty).	
	Access	Read-only	
Examples	<pre>1 Create a model object. modelObj = sbiome</pre>	odel ('my_model');	
	<b>2</b> Add reaction objects.		
	reactionObj = add	dreaction (modelObj, 'a + b -> c + d');	
	<b>3</b> Verify the assignment	t.	
	<pre>productsObj = get(reactionObj, 'Products') MATLAB returns:</pre>		
	SimBiology Specie	es Array	
	Index: Compartme	ent: Name: InitialAmount: InitialAmountUnits:	

## **Products**

1	unnamed	С	0
2	unnamed	d	0

See Also	addkineticlaw, add	dproduct, addspecies	, rmproduct
----------	--------------------	----------------------	-------------

#### **Purpose** Set random number generator

## **Description** The RandomState property sets the random number generator for the stochastic solvers. It is a property of the SolverOptions object. SolverOptions is a property of the configset object.

SimBiology software uses a pseudorandom number generator. The sequence of numbers generated is determined by the state of the generator, which can be specified by the integer RandomState. If RandomState is set to integer J, the random number generator is initialized to its  $J^{th}$  state. The random number generator can generate all the floating-point numbers in the closed interval  $[2^{(-53)}, 1-2^{(-53)}]$ . Theoretically, it can generate over  $2^{1492}$  values before repeating itself. But for a given state, the sequence of numbers generated will be the same. To change the sequence, change RandomState. SimBiology software resets the state at startup. The default value of RandomState is [].

#### **Characteristics**

Applies to	Objects: SolverOptions impltau	for SSA,	expltau,
Data type	int		
Data values	Default is [] (empty).		
Access	Read/write		

#### **Examples** This example shows how to change RandomState settings.

 Retrieve the configset object from the modelObj and change the SolverType to expltau.

modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj); set(configsetObj, 'SolverType', 'expltau')

**2** Change the Randomstate to 5.

See Also

```
set(configsetObj.SolverOptions, 'RandomState', 5);
get(configsetObj.SolverOptions, 'RandomState'))
ans =
5
ErrorTolerance, LogDecimation, MaxIterations
```

#### Purpose Array of reaction reactants

**Description** The Reactants property is a 1-by-n species object array of reactants in the reaction. If the Reaction property is modified to use a different reactant, the Reactants property will be updated accordingly.

You can add reactant species to the reaction with the addreactant method.

You can remove reactant species from the reaction with the rmreactant method. You can also update reactants by setting the Reaction property with the function set.

#### **Characteristics**

cital acterizines					
	Applies to	Object: reaction			
	Data type	Species object of	r array of species o	bjects	
	Data values	Species objects.	Default is [] (emp	oty).	
	Access	Read-only			
Examples	1 Create a model obj		do]');		
	moderobj – Sb.	iomodel ('my_mo	der);		
	<b>2</b> Add reaction objects.				
	reactionObj =	addreaction (m	odelObj, 'a + b	-> c + d');	
	<b>3</b> View the reactants	for reactionObj			
<pre>get(reactionObj, 'Reactants')</pre>					
	MATLAB returns:				
	SimBiology Species Array				
	Index: Compar 1 unnar	rtment: Name: ned a	InitialAmount: 0	InitialAmountUnits:	

## Reactants

0	0
(	(

**See Also** addreactant, addreaction, addspecies, rmreactant

#### PurposeReaction object reaction

**Description** Property to indicate the reaction represented in the reaction object. Indicates the chemical reaction that can change the amount of one or more species, for example, 'A + B > C'. This property is different from the model object property called Reactions.

See addreaction for more information on how the  $\ensuremath{\mathsf{Reaction}}$  property is set.

#### **Characteristics**

Object: reaction
char string
Valid reaction string. Default is ' ' (empty).
Read/write

#### **Examples** 1 Create a model object, and then add a reaction object.

modelObj = sbiomodel ('my\_model'); reactionObj = addreaction (modelObj, 'a + b -> c + d');

**2** Verify that the reaction property records the input.

get (reactionObj, 'Reaction')

MATLAB returns:

ans =

a + b -> c + d

**See Also** addreaction, sbioreaction

## ReactionRate

**Purpose** Reaction rate equation in reaction object

### **Description** Th

The ReactionRate property defines the reaction rate equation. You can define a ReactionRate with or without the KineticLaw property. KineticLaw defines the type of reaction rate. The addkineticlaw function configures the ReactionRate based on the KineticLaw and the species and parameters specified in the kinetic law object properties SpeciesVariableNames and ParameterVariableNames.

The reaction takes place in the reverse direction if the Reversible property is true. This is reflected in ReactionRate. The ReactionRate includes the forward and reverse rate if reversible.

You can specify ReactionRate without KineticLaw. Use the set function to specify the reaction rate equation. SimBiology software adds species variables while creating reactionObj using the addreaction method. You must add the parameter variables (to the modelObj in this case). See the example below.

After you specify the ReactionRate without KineticLaw and you later configure the reactionObj to use KineticLaw, the ReactionRate is unset until you specify SpeciesVariableNames and ParameterVariableNames.

#### **Characteristics**

Applies to	Object: reaction
Data type	char string
Data values	Reaction rate string. Default is ' ' (empty).
Access	Read/write

#### Examples Example 1

Create a model, add a reaction, and assign the expression for the reaction rate equation.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

2 Create a kinetic law object for the reaction object of the type 'Henri-Michaelis-Menten'.

kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');

reactionObj KineticLaw property is configured to kineticlawObj.

3 The 'Henri-Michaelis-Menten' kinetic law has two parameter variables (Vm and Km) and one species variable (S) that you should set. To set these variables, first create the parameter variables as parameter objects (parameterObj1, parameterObj2) with names Vm\_d and Km\_d and assign them to kineticlawObj.

```
parameterObj1 = addparameter(kineticlawObj, 'Vm_d');
parameterObj2 = addparameter(kineticlawObj, 'Km_d');
```

4 Set the variable names for the kinetic law object.

```
set(kineticlawObj,'ParameterVariableNames', {'Vm_d' 'Km_d'});
set(kineticlawObj,'SpeciesVariableNames', {'a'});
```

5 Verify that the reaction rate is expressed correctly in the reaction object ReactionRate property.

get (reactionObj, 'ReactionRate')

MATLAB returns:

ans =

 $Vm_d*a/(Km_d + a)$ 

#### **Example 2**

Create a model, add a reaction, and specify ReactionRate without a kinetic law.

1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a + b -> c + d');
```

2 Specify ReactionRate and verify the assignment.

```
set (reactionObj, 'ReactionRate', 'k*a');
get(reactionObj, 'ReactionRate')
```

MATLAB returns:

ans =

k\*a

**3** You cannot simulate the model until you add the parameter k to the modelObj.

parameterObj = addparameter(modelObj, 'k');

SimBiology adds the parameter to the modelObj with default Value = 1.0 for the parameter.

See Also addparameter, addreaction, Reversible, sbioparameter, sbioreaction

## **Reactions**

#### Purpose Array of reaction objects

#### Description Property to indicate the reactions in a Model object. Read-only array of reaction objects.

A reaction object defines a chemical reaction that occurs between species. The species for the reaction are defined in the Model object property Species.

You can add a reaction to a model object with the method addreaction, and you can remove a reaction from the model object with the method delete.

#### **Characteristics**

cital acterizites		
	Applies to	Object: model
	Data type	Array of reaction objects
	Data values	Reaction object
	Access	Read-only
Example	<pre>I Create a model object, and then add a reaction object. modelObj = sbiomodel ('my_model'); reactionObj = addreaction (modelObj, 'a + b -&gt; c + d');</pre>	
	2 Verify that the reaction get (modelObj, 'F	ns property records the input. Reactions')
	MATLAB returns:	
SimBiology Reaction Array		ion Array
	Index: React: 1 a + b	ion: -> c + d
See Also	addreaction, delete, sb	ioreaction

## RelativeTolerance

Purpose	Specify allowable error relative to component	
Description	The RelativeTolerance property specifies the allowable error tolerance relative to the state vector at each simulation step. The state vector contains values for all the state variables, for example, species amounts for all the species.	
	RelativeTolerance is a property of the SolverOptions object. SolverOptions is a property of the configset object. RelativeTolerance is available for the ode solvers ('ode45', 'ode23', 'ode113', 'ode15s', 'ode23s', 'ode23t', and 'ode23tb').	
	If you set the RelativeTolerance at 1e-2, you are specifying that an error of 1% relative to each state value is acceptable at each simulation step.	
	At each simulation step, the solver estimates the local error $e_i$ in the ith state vector y. Simulation converges at that time step if $e_i$ satisfies the following equation:	
	$ e_i  \le \max(\text{RelativeTolerance} *  y_i , AbsoluteTolerance)$	
	Thus at higher state values, convergence is determined by RelativeTolerance. As the state values approach zero, convergence is controlled by AbsoluteTolerance. The choice of values for RelativeTolerance and AbsoluteTolerance will vary depending on the problem. The default values should work for first trials of the simulation; however if you want to optimize the solution, consider that there is a trade-off between speed and accuracy. If the simulation takes too long, you can increase the values of RelativeTolerance and AbsoluteTolerance at the cost of some accuracy. If the results appear to be inaccurate, you can decrease the tolerance values but this will slow down the solver. If the magnitude of the state values is high, you can try to decrease the relative tolerance to get more accurate results.	
Characteristics		

Applies toObject: SolverOptionsData typedouble

	Data values	>0, <1. Default is 1e-3.	
	Access	Read/write	
Examples	<pre>This example shows how to change AbsoluteTolerance. 1 Retrieve the configset object from the modelObj. modelObj = sbiomodel('cell');</pre>		
	configsetObj = (	jetconfigset(modelObj)	
	<b>2</b> Change the AbsoluteTolerance to 1e-8.		
		.SolverOptions, 'RelativeTolerance', 1.0e-6); .SolverOptions, 'RelativeTolerance')	
	ans =		
	1.0000e-006		
See Also	AbsoluteTolerance		

## Reversible

#### **Purpose** Specify whether reaction is reversible or irreversible

**Description** The Reversible property defines whether a reaction is reversible or irreversible. The rate of the reaction is defined by the ReactionRate property. For a reversible reaction, the reaction rate equation is the sum of the rate of the forward and reverse reactions. The type of reaction rate is defined by the KineticLaw property. If a reaction is changed from reversible to irreversible or vice versa after KineticLaw is assigned, the new ReactionRate is determined only if Type is MassAction. All other Types result in unchanged ReactionRate. For MassAction, the first parameter specified is assumed to be the rate of the forward reaction.

#### **Characteristics**

Applies to	Object: reaction
Data type	boolean
Data values	true, false. Default value is false.
Access	Read/write

## **Examples** Create a model, add a reaction, and assign the expression for the reaction rate equation.

1 Create model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

**2** Set the Reversible property for the reactionObj to true and verify this setting.

```
set (reactionObj, 'Reversible', true)
get (reactionObj, 'Reversible')
```

MATLAB returns:

ans =

1

MATLAB returns 1 for true and 0 for false.

In the next steps the example illustrates how the reaction rate equation is assigned for reversible reactions.

**3** Create a kinetic law object for the reaction object of the type 'MassAction'.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

reactionObj KineticLaw property is configured to kineticlawObj.

4 The 'MassAction' kinetic law for reversible reactions has two parameter variables ('Forward Rate Parameter' and 'Reverse Rate Parameter') that you should set. The species variables for MassAction are automatically determined. To set the parameter variables, first create the parameter variables as parameter objects (parameterObj1, parameterObj2) named Kf and Kr and assign the object to kineticlawObj.

```
parameterObj1 = addparameter(kineticlawObj, 'Kf');
parameterObj2 = addparameter(kineticlawObj, 'Kr');
```

5 Set the variable names for the kinetic law object.

```
set(kineticlawObj, 'ParameterVariableNames', {'Kf' 'Kr'});
```

6 Verify that the reaction rate is expressed correctly in the reaction object ReactionRate property.

get (reactionObj, 'ReactionRate')

MATLAB returns:

ans =

Kf\*a\*b - Kr\*c\*d

**See Also** addparameter, addreactant, addreaction, ParameterVariableNames, ReactionRate, sbioreaction

#### **Purpose** Specify species and parameter interactions

**Description** The Rule property contains a rule that defines how certain species and parameters should interact with one another. For example, a rule could state that the total number of species A and species B must be some value. Rule is a MATLAB expression that defines the change in the species object quantity or a parameter object Value when the rule is evaluated.

You can add a rule to a model object with the addrule method and remove the rule with the delete method. For more information on rules, see addrule and RuleType.

#### **Characteristics**

	Applies to	Object: rule	
	Data type	char string	
	Data values	char string defined as species or parameter objects. Default is empty.	
	Access	Read/write	
Example	1 Create a model	object, and then add a reaction object.	
	-	<pre>modelObj = sbiomodel ('my_model'); reactionObj = addreaction (modelObj, 'a + b -&gt; c + d');</pre>	
	<b>2</b> Add a rule.		
	ruleObj = a	addrule(modelObj, '10-a+b')	
	MATLAB returns:		
	SimBiology	Rule Array	
		RuleType: Rule: algebraic 10-a+b	

See Also addrule, delete, sbiorule

#### **Purpose** Specify type of rule for rule object

# **Description** The RuleType property indicates the type of rule defined by the rule object. A Rule object defines how certain species, parameters, and compartments should interact with one another. For example, a rule could state that the total number of species A and species B must be some value. Rule is a MATLAB expression that defines the change in the species object quantity or a parameter object Value when the rule is evaluated.

You can add a rule to a model object with the addrule method and remove the rule with the delete method. For more information on rules see addrule.

The types of rules in SimBiology are as follows:

- initialAssignment Lets you specify the initial value of a parameter, species, or compartment capacity, as a function of other model component values in the model.
- repeatedAssignment Lets you specify a value that holds at all times during simulation, and is a function of other model component values in the model.
- algebraic Lets you specify mathematical constraints on one or more parameters, species, or compartments that must hold during a simulation.
- rate Lets you specify the time derivative of a parameter value, species amount, or compartment capacity.

#### **Constraints on Varying Species Using a Rate Rule**

If the model has a species defined in concentration, being varied by a rate rule, and it is in a compartment with varying volume, you can only use rate or initialAssignment rules to vary the compartment volume.

Conversely, if you are varying a compartment's volume using a repeatedAssignment or algebraic rules, then you cannot vary a species (defined in concentration) within that compartment, with a rate rule.

The reason for these constraints is that, if a species is defined in concentration and it is in a compartment with varying volume, the time derivative of that species is a function of the compartment's rate of change. For compartments varied by rate rules, the solver has that information.

Note that if you specify the species in amounts there are no constraints.

#### **Characteristics**

Applies to	Object: rule
Data type	char string
Data values	'algebraic', 'assignment', 'rate'. Default value is 'assignment'.
Access	Read/write

**Examples** 1 Create a model object, and then add a reaction object.

```
modelObj = sbiomodel ('my_model');
reactionObj = addreaction (modelObj, 'a -> b');
```

**2** Add a rule that specifies the quantity of a species c. In the rule expression, k is the rate constant for a -> b.

ruleObj = addrule(modelObj, 'c = k\*(a+b)')

**3** Change the RuleType from the default ('algebraic') to 'rate' and verify it using the get command.

```
set(ruleObj, 'RuleType', 'rate');
get(ruleObj)
```

MATLAB returns all the properties for the rule object.

Active: 1 Annotation: '' Name: '' Notes: ''

```
Parent: [1x1 SimBiology.Model]
Rule: 'c = k*(a+b)'
RuleType: 'rate'
Tag: ''
Type: 'rule'
UserData: []
```

**See Also** "Changing Model Component Values Using Rules" in the *SimBiology User's Guide*, addrule, delete, sbiorule

# Rules

Purpose	Array of rules in model object		
Description	The Rules property shows the rules in a Model object. Read-only array of SimBiology.Rule objects.		
	A <i>rule</i> is a mathematical expression that modifies a species amount or a parameter value. A rule defines how certain species and parameters should interact with one another. For example, a rule could state that the total number of species A and species B must be some value.		
	You can add a rule to a model object with the addrule method and remove the rule with the delete method. For more information on rules, see addrule and RuleType.		
Characteristics			
	Applies to	Object: model	
	Data type	Array of rule objects	
	Data values	Rule object	
	Access	Read-only	
Examples	<pre>I Create a model object, and then add a reaction object. modelObj = sbiomodel ('my_model'); reactionObj = addreaction (modelObj, 'a + b -&gt; c + d');</pre>		
	<b>2</b> Add a rule.		
	<pre>ruleobj = addrule(modelObj, '10-a+b')</pre>		
	MATLAB returns:		
	SimBiology Rule Array		
	Index: RuleType: 1 algebraic	Rule: 10-a+b	
See Also	addrule, delete, sbiorule		

#### **Purpose** Information about simulation

# **Description** The RunInfo property contains information describing the simulation run that yielded the data in the SimData object.

The following information is stored:

- Configset A struct form of the configuration set used during simulation. This would typically be the model's active configset.
- Variant A struct form of the variant(s) used during simulation.
- SimulationDate The date/time of simulation.
- SimulationType Either 'single run' or 'ensemble run', depending on whether the data object was created using the function sbiosimulate or the function sbioensemblerun.

#### **Characteristics**

	Applies to	Object: SimData
	Data type	struct
	Data values	Default values are as follows:
		ConfigSet: [] SimulationDate: '' SimulationType: '' Variant: [] In practice, the ConfigSet, SimulationDate, and SimulationType fields are rarely empty, since they are
	Access	populated after simulation. Read-only
See Also	StopTime, StopTimeType	

# **RuntimeOptions**

Purpose	Options for logged species	
Description	The RuntimeOptions property holds options for species that will be logged during the simulation run. The run-time options object can be accessed through this property.	
	The LogDecimation property of the configuration set object defines how often data is logged.	
Property	StatesToLog	Specify species data recorded
Summary	Туре	Display top-level SimBiology object type
Characteristics	Applies to	Object: configset
	Data type	Object. com igset
	Data values	Run-time options
	Access	Read-only
Examples	<pre>I Create a model object, and retrieve its configuration set. modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj);</pre>	
	<b>2</b> Retrieve the RuntimeOptions object from the configset object.	
	runtimeObj = get(configsetObj, 'RunTimeOptions') Runtime Settings:	
	StatesToLog:	all
See Also	MATLAB functions get, set	

#### **Purpose** Enable or disable sensitivity analysis

**Description** The SensitivityAnalysis property lets you compute the time-dependent sensitivities of all the species states defined by the StatesToLog property with respect to the SpeciesInputFactors and the ParameterInputFactors that you specify in the SensitivityAnalysisOptions property of the configuration set object.

SensitivityAnalysis is a property of the SolverOptions object. SolverOptions is a property of the configuration set object. SensitivityAnalysis is available for the ode solvers ('ode45', 'ode23', 'ode113', 'ode15s', 'ode23s', 'ode23t', and 'ode23tb').

See SensitivityAnalysisOptions for more information on setting up sensitivity analysis. See "Sensitivity Analysis" in the SimBiology User's Guide documentation for a description of sensitivity analysis calculations.

#### **Characteristics**

Applies to	Object: SolverOptions
Data type	logical
Data values	1, 0, true, false. Default is false.
Access	Read/write

#### **Examples** This example shows how to enable SensitivityAnalysis.

1 Retrieve the configset object from the modelObj.

modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj);

**2** Enable SensitivityAnalysis.

```
set(configsetObj.SolverOptions, 'SensitivityAnalysis', true);
get(configsetObj.SolverOptions, 'SensitivityAnalysis')
```

# **SensitivityAnalysis**

ans =

on

# See Also SensitivityAnalysisOptions, SolverOptions, SolverType, StatesToLog

#### **Purpose** Specify sensitivity analysis options

**Description** The SensitivityAnalysisOptions property is an object that holds the sensitivity analysis options in the configuration set object. Sensitivity analysis is only supported for deterministic (ODE) simulations.

Properties of SensitivityAnalysisOptions are summarized in "Property Summary" on page 6-114.

When sensitivity analysis is enabled, the following command

[t,x,names] = sbiosimulate(modelObj)

returns [t,x,names], where

- t is an n-by-1 vector, where n is the number of steps taken by the ode solver and t defines the time steps of the solver.
- x is an n-by-m matrix, where n is the number of steps taken by the ode solver and m is:

Number of states specified in StatesToLog + (Number of species specified in StatesToLog\*Number of input factors)

A SimBiology state includes species and nonconstant parameters.

• names is the list of states logged and the list of sensitivities of the species specified in StatesToLog with respect to the input factors.

For an example of the output, see "Examples" on page 6-114.

You can add a number of configuration set objects with different SensitivityAnalysisOptions to the model object with the addconfigset method. Only one configuration set object in the model object can have the Active property set to true at any given time.

Property Summary	Normalization ParameterInputFactor SpeciesInputFactors	rs	Specify normalization type for sensitivity analysis Specify parameter input factors for sensitivity analysis Specify species inputs for sensitivity analysis
	SpeciesOutputs		Specify species outputs for sensitivity analysis
Characteristics	Applies to	Object: co	nfiguration set
	Data type	Object	
	Data values	Sensitivi	ityAnalysisOptions properties as ed in "Property Summary" on page
	Access	Read-only	
Examples	This example shows how to set SensitivityAnalysisOptions.		sitivityAnalysisOptions.
	1 Import the radio deca	y model from	m SimBiology demos.
	<pre>modelObj = sbmlimport('radiodecay');</pre>		adiodecay');
	<b>2</b> Retrieve the configset object from the modelObj.		om the modelObj.
	<pre>configsetObj = getconfigset(modelObj);</pre>		et(modelObj);
	<b>3</b> Add a parameter to the ParameterInputFactors property and display. Use the sbioselect function to retrieve the parameter object from the model.		
			ysisOptions,'ParameterInputFactors', 'parameter', 'Name', 'c'));

get (configsetObj.SensitivityAnalysisOptions, 'ParameterInputFactors') SimBiology Parameter Array Index: Name: Value: ValueUnits: 1 С 0.5 1/second 4 Add a species to the SpeciesInputFactors property and display. Use the sbioselect function to retrieve the species object from the model. set(configsetObj.SensitivityAnalysisOptions,'SpeciesInputFactors', ... sbioselect(modelObj,'Type', 'species', 'Name', 'z')); get (configsetObj.SensitivityAnalysisOptions, 'SpeciesInputFactors'); set(configsetObj.SensitivityAnalysisOptions, ... 'SpeciesOutputs', sbioselect(modelObj, 'Type', 'species')); **5** Enable SensitivityAnalysis. set(configsetObj.SolverOptions, 'SensitivityAnalysis', true); get(configsetObj.SolverOptions, 'SensitivityAnalysis')

```
ans =
1
```

**6** Simulate and return the results to three output variables. See "Description" on page 6-113 for more information.

[t,x,names] = sbiosimulate(modelObj);

7 Display the names.

names names = 'x' 'z' 'd[x]/d[z]\_0' 'd[z]/d[z]\_0' 'd[x]/d[c]' 'd[z]/d[c]'

**8** Display state values x.

Х

The display follows the column order shown in names for the values in x. The rows correspond to t.

See Also addconfigset, getconfigset

Purpose	Specify model solver options	
Description	The SolverOptions property is an object that holds the model solve options in the configset object. Changing the property SolverType changes the options specified in the SolverOptions object. Properties of SolverOptions are summarized in "Property Summar on page 6-117.	
Property Summary	AbsoluteTolerance	Specify largest allowable absolute error
	ErrorTolerance	Specify explicit or implicit tau error tolerance
	LogDecimation	Specify recorded simulation output frequency
	MaxIterations	Specify nonlinear solver maximum iterations in implicit tau
	MaxStep	Specify upper bound on solver step size
	RandomState	Set random number generator
	RelativeTolerance	Specify allowable error relative to component
	SensitivityAnalysis	Enable or disable sensitivity analysis
	Туре	Display top-level SimBiology object type

#### **Characteristics**

Applies to	Object: configset
Data type	Object

```
Data values
                                         Solver options depending on SolverType.
                                         Default is SolverOptions for default
                                         SolverType (ode15s).
                   Access
                                         Read-only
Examples
                  This example shows the changes in SolverOptions for various
                  SolverType settings.
                  1 Retrieve the configset object from the modelObj.
                       modelObj = sbiomodel('cell');
                       configsetObj = getconfigset(modelObj);
                  2 Configure the SolverType to ode45.
                       set(configsetObj, 'SolverType', 'ode45');
                       get(configsetObj, 'SolverOptions')
                       Solver Settings: (ode)
                            AbsoluteTolerance:
                                                    1.000000e-006
                            RelativeTolerance:
                                                    1.000000e-003
                  3 Configure the SolverType to ssa.
                       set(configsetObj, 'SolverType', 'ssa');
                       get(configsetObj, 'SolverOptions')
                       Solver Settings: (ssa)
                            LogDecimation:
                                                    1
                            RandomState:
                                                    []
                  4 Configure the SolverType to impltau.
```

```
set(configsetObj, 'SolverType', 'impltau');
                      get(configsetObj, 'SolverOptions')
                      Solver Settings: (impltau)
                           ErrorTolerance:
                                                  3.000000e-002
                           LogDecimation:
                                                  1
                           AbsoluteTolerance:
                                                  1.000000e-002
                           RelativeTolerance:
                                                  1.000000e-002
                           MaxIterations:
                                                  15
                           RandomState:
                                                  []
                  5 Configure the SolverType to expltau.
                      set(configsetObj, 'SolverType', 'expltau');
                      get(configsetObj, 'SolverOptions')
                      Solver Settings: (expltau)
                           ErrorTolerance:
                                                  3.000000e-002
                           LogDecimation:
                                                  1
                           RandomState:
                                                  []
See Also
                 addconfigset, getconfigset
```

# SolverType

Purpose	Select solver type for simulation
---------	-----------------------------------

**Description** The SolverType property lets you specify the solver to use for a simulation. The valid SolverType values are 'ssa', 'expltau', 'impltau', 'ode45', 'ode23', 'ode113', 'ode15s', 'ode23s', and 'ode23t'. The default solver is ode15s. For a discussion about these solver types, see "Selecting a Solver" in the SimBiology User's Guide documentation.

Changing the solver type changes the options (properties) specified in the SolverOptions property of the configset object. If you change any SolverOptions, these changes are persistent when you switch SolverType. For example, if you set the ErrorTolerance for the expltau solver and then change to impltau when you switch back to expltau, the ErrorTolerance will have the number you assigned.

#### **Characteristics**

	Applies to	Object: configset
	Data type	enum
	Data values	'ssa', 'expltau', 'impltau', 'ode45', 'ode23', 'ode113', 'ode15s', 'ode23s', 'ode23t', 'ode23tb'. Default is ode15s.
	Access	Read/write
Examples	<pre>amples 1 Retrieve the configset object from the mode modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelOb</pre>	
	Configuration Settings - default (active) SolverType: ode15s StopTime: 10.000000	
	Solver0ptio	ns:

### SolverType

AbsoluteTolerance: 1.000000e-006 RelativeTolerance: 1.000000e-003 RuntimeOptions: StatesToLog: all CompileOptions: UnitConversion: true DimensionalAnalysis: true 2 Configure the SolverType to ode45. set(configsetObj, 'SolverType', 'ode45') configset0bj Configuration Settings - default (active) SolverType: ode45 StopTime: 10.000000 SolverOptions: AbsoluteTolerance: 1.000000e-006 1.000000e-003 RelativeTolerance: RuntimeOptions: StatesToLog: all CompileOptions: UnitConversion: true DimensionalAnalysis: true

See Also getconfigset, set

# **Species**

Purpose	Array of species in compartment object		
Description	The Species property is a property of the compartment object and indicates all the species in a compartment object. Species is a read-only array of SimBiology species objects.		
	In the model object, Species contains a flat list of all the species that exist within all the compartments in the model. You should always access a species through its compartment rather than the model object. Use the format <i>compartmentName.speciesName</i> , for example, nucleus.DNA. Another example of the syntax is modelObj.Compartments(2).Species(1). The Species property in the model object might not be available in a future version of the software.		
	Species are entities that take part in reactions. A species object is added to the Species property when a reaction is added to the model object with the method addreaction. A species object can also be added to the Species property with the method addspecies.		
	If you remove a reaction with the method delete, and a species is no longer being used by any of the remaining reactions, the species object is <i>not</i> removed from the Species property. You have to use the delete method to remove species.		
	There are reserved characters that cannot be used in species object names. See Name for more information.		
Characteristics			
	Applies to     Object: compartment       Data turns     Arrow of ansaiss shipets		
	Data type Array of species objects		
	Data values Species object. Default is [] (empty).		
	Access	Read-only	
See Also	addcompartment, addreaction, addspecies, delete		

#### **Purpose** Specify species inputs for sensitivity analysis

**Description** Use the SpeciesInputFactors property to specify the species with respect to which you want to compute the sensitivities of the species states in your model.

SpeciesInputFactors is a property of the SensitivityAnalysisOptions object. SenstivityAnalysisOptions is a property of the configuration set object.

The SimBiology software calculates sensitivities with respect to the initial amounts of the species specified in this property. When you simulate a model with SensitivityAnalysis enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species specified in StatesToLog. For a description of the output, see the SensitivityAnalysisOptions property description.

#### **Characteristics**

Applies to	Object: SensitivityAnalysisOptions
Data type	Species object or array of species objects
Data values	Species object array. Default is [] (empty).
Access	Read/write

**Examples** This example shows how to set SpeciesInputFactors for sensitivity analysis.

1 Import the radio decay model from the SimBiology demos.

modelObj = sbmlimport('radiodecay');

**2** Retrieve the configuration set object from modelObj.

configsetObj = getconfigset(modelObj);

**3** Add a species to the SpeciesInputFactors property and display. Use the sbioselect function to retrieve the species object from the model.

set(configsetObj.SensitivityAnalysisOptions,'SpeciesInputFactors', ... sbioselect(modelObj, 'Type', 'species', 'Name', 'z')); get (configsetObj.SensitivityAnalysisOptions, 'SpeciesInputFactors')

SimBiology Species Array

Index: Compartment: Name: InitialAmount: InitialAmountUnits: 1 unnamed z 0 molecule

See Also ParameterInputFactors, sbioselect, SensitivityAnalysis, SensitivityAnalysisOptions

#### **Purpose** Specify species outputs for sensitivity analysis

# **Description** The SpeciesOutputs property allows you to specify the species for which you want to compute sensitivities. SpeciesOutputs is a property of the SensitivityAnalysisOptions object. SenstivityAnalysisOptions is a property of the configuration set object.

The SimBiology software calculates sensitivities with respect to the values of the parameters specified in ParameterInputFactors and the initial amounts of the species specified in SpeciesInputFactors. When you simulate a model with SensitivityAnalysis enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species specified in SpeciesOutputs. For a description of the output, see the SensitivityAnalysisOptions property description.

#### **Characteristics**

Applies to	$\operatorname{Object}:$ SensitivityAnalysisOptions
Data type	Species object or array of species objects
Data values	Species object array. Default is [] (empty).
Access	Read/write

#### **Examples** This example shows how to set SpeciesOutputs for sensitivity analysis.

1 Import the radio decay model from the SimBiology demos.

modelObj = sbmlimport('radiodecay');

2 Retrieve the configuration set object from modelObj.

configsetObj = getconfigset(modelObj);

**3** Add a species to the SpeciesOutputs property and display. Use the sbioselect function to retrieve the species object from the model.

set(configsetObj.SensitivityAnalysisOptions,'SpeciesOutputs', ... sbioselect(modelObj, 'Type', 'species', 'Name', 'z')); get (configsetObj.SensitivityAnalysisOptions, 'SpeciesOutputs')

SimBiology Species Array

Index: Compartment: Name: InitialAmount: InitialAmountUnits: 1 unnamed z 0 molecule

**See Also** ParameterInputFactors, sbioselect, SensitivityAnalysis, SensitivityAnalysisOptions, SpeciesInputFactors

#### **Purpose** Cell array of species used in reaction rate equation

# **Description** The SpeciesVariableNames property shows the species used by the kinetic law object to determine the ReactionRate equation in the reaction object. Use setspecies to assign SpeciesVariableNames. When you assign species to SpeciesVariableNames, SimBiology software maps these species names to SpeciesVariables in the kinetic law object.

The ReactionRate property of a reaction object shows the result of a mapping from an abstract kinetic law. The ReactionRate is determined by the kinetic law object Expression property by mapping ParameterVariableNames to ParameterVariables and SpeciesVariableNames to SpeciesVariables.

#### **Characteristics**

Applies to	Object: kinetic law
Data type	Cell array of strings
Data values	Cell array of species names
Access	Read/write

# **Examples** Create a model, add a reaction, and assign the SpeciesVariableNames for the reaction rate equation.

1 Create a model object, and then add a reaction object.

modelObj = sbiomodel('my\_model'); reactionObj = addreaction(modelObj, 'a -> c + d');

2 Create a kinetic law object for the reaction object, of the type 'Henri-Michaelis-Menten'

kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');

The reactionObj KineticLaw property is configured to kineticlawObj.

3 The 'Henri-Michaelis-Menten' kinetic law has one species variable (S) that you should set. To set this variable:

```
setspecies(kineticlawObj,'S', 'a');
```

**4** Verify that the species variable is correct.

```
get (kineticlawObj, 'SpeciesVariableNames')
```

MATLAB returns:

```
ans =
'a'
```

See Also Expression, ParameterVariables, ParameterVariableNames, ReactionRate, setparameter, SpeciesVariables

#### Purpose Species in abstract kinetic law

**Description** This property shows species variables that are used in the Expression property of the kinetic law object to determine the ReactionRate equation in the reaction object. Use the MATLAB function set to assign SpeciesVariables to an abstract kinetic law. For more information, see abstract kinetic law.

#### **Characteristics**

Applies to	Objects: abstract kinetic law, kineticlaw
Data type	Cell array of strings
Data values	Defined by abstract kinetic law
Access	Read/write in abstract kinetic law. Read-only in kinetic law.

**Examples** Create a model, add a reaction, and assign the SpeciesVariableNames for the reaction rate equation.

**1** Create a model object, and then add a reaction object.

```
modelObj = sbiomodel('my_model');
reactionObj = addreaction(modelObj, 'a -> c + d');
```

2 Create a kinetic law object for the reaction object, of the type 'Henri-Michaelis-Menten'.

kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');

reactionObj KineticLaw property is configured to kineticlawObj.

3 View the species variable for 'Henri-Michaelis-Menten' kinetic law.

get (kineticlawObj, 'SpeciesVariables')

MATLAB returns:

# **SpeciesVariables**

ans = 'S'

See Also Expression, ParameterVariables, ParameterVariableNames, ReactionRate, set, setparameter, SpeciesVariableNames

Purpose Specif	y species	data	recorded
----------------	-----------	------	----------

**Description** The StatesToLog property indicates the species data to log during a simulation. This is the data returned in x during execution of (t,x) = sbiosimulate(modelObj). By default all species are logged.

#### **Characteristics**

Applies to	Object: RunTimeOptions
Data type	Object or vector of objects
Data values	Species objects to log. Default is All.
Access	Read/write

**Examples** This example shows how to assign species to StatesToLog.

1 Create a model object by importing the file oscillator.xml.

modelObj = sbmlimport('oscillator');

2 Retrieve the first and second species in modelObj.

speciesObj1 = modelObj.Species(1); speciesObj2 = modelObj.Species(2);

3 Retrieve the configsetObj of modelObj.

configsetObj = getconfigset(modelObj);

**4** Set the StatesToLog to record three species: two using the retrieved species objects and one using indexing and view the species in StatesToLog.

```
set (configsetObj.RuntimeOptions, 'StatesToLog', ...
[speciesObj1, speciesObj2, modelObj.Species(3)]);
get(configsetObj.RuntimeOptions, 'StatesToLog')
```

### **Stoichiometry**

<b>FUIPOSE</b> Species coefficients in reaction	Purpose	Species coefficients in reaction
---	---------	----------------------------------

# **Description** The Stoichiometry property specifies the species coefficients in a reaction. Enter an array of doubles indicating the stoichiometry of reactants (negative value) and products (positive value). Example: [-1 -1 2].

The double specified cannot be 0. The reactants of the reaction are defined with a negative number. The products of the reaction are defined with a positive number. For example, the reaction 3 H + A-> 2 C + F has the Stoichiometry value of [-3 -1 2 1].

When this property is configured, the Reaction property updates accordingly. In the above example, if the Stoichiometry value was set to  $[-2 - 1 \ 2 \ 3]$ , the reaction is updated to 2H + A -> 2C + 3F.

The length of the Stoichiometry array is the sum of the Reactants array and the Products array. To remove a product or reactant from a reaction, use the rmproduct or rmreactant function. Add a product or reactant and set stoichiometry with methods addproduct and addreactant

ODE solvers support double stoichiometry values such as 0.5. Stochastic solvers and dimensional analysis currently support only integers in Stoichiometry, therefore you must balance the reaction equation and specify integer values for these two cases.

A -> null has a stoichiometry value of [-1]. null -> B has a stoichiometry value of [1].

#### **Characteristics**

Applies to	Object: reaction
Data type	Double array
Data values	1-by-n double, where n is length (products) + length (reactants). Default [] (empty).
Access	Read/write

```
Examples
                  1 Create a reaction object.
                       modelObj = sbiomodel('cell');
                       reactionObj = addreaction(modelObj, '2 a + 3 b -> d + 2 c');
                  2 Verify the Reaction and Stoichiometry properties for reactionObj.
                       get(reactionObj, 'Stoichiometry')
                    MATLAB returns:
                       ans =
                       -2 -3 1 2
                  3 Set stoichiometry to [-1 -2 2 2].
                       set (reactionObj, 'Stoichiometry', [-1 -2 2 2]);
                       get (reactionObj, 'Stoichiometry')
                    MATLAB returns:
                       ans =
                        - 1
                              -2
                                     2
                                           2
                  4 Note with get that the Reaction property updates automatically.
                      get (reactionObj, 'Reaction')
                    MATLAB returns:
                      ans =
                      a + 2 b -> 2 d + 2 c
See Also
                  addproduct, addreactant, addreaction, Reaction, rmproduct,
                  rmreactant
```

# **StopTime**

Purpose	Set stop time for simulation	
Description	The StopTime property sets the stop time for a simulation. The type of StopTime is specified in the property StopTimeType.	
Characteristics	Applies to Data type Data values Access	Object: configset double Enter a positive number. Default is 10. Read/write
Examples	<pre>1 Retrieve the configset object from modelObj. modelObj = sbiomodel('cell'); configsetObj = getconfigset(modelObj) 2 Configure the StopTime to 20. set(configsetObj, 'StopTime', 20) get(configsetObj, 'StopTime') ans = 20</pre>	
See Also	StopTimeType, Time	Jnits

#### **Purpose** Specify type of stop time for simulation

# **Description** The StopTimeType property sets the type of stop time for a simulation. The stop time is specified in the StopTime property of the configset object. Valid types are approxWallTime, numberOfLogs, and simulationTime. The default is simulationTime.

- simulationTime Specify the stop time for the simulation. The solver determines and sets the time steps and the simulation stops when it reaches the specified StopTime.
- approxWallTime Specify the approximate stop time according to the clock. For example,10s of approxWallTime is approximately 10s of real time.
- numberOfLogs Specify the total number of simulation steps to be recorded during the simulation. For example if you want to log three simulation steps, the numberOfLogs is 3. The simulation will stop after the specified numberOfLogs.

You can change the StopTimeType setting with the set function.

#### **Characteristics**

	Applies to	Object: configset
	Data type	enum
	Data values	approxWallTime, numberOfLogs, and simulationTime
	Access	Read/write
Examples	<b>1</b> Retrieve the configset object from modelObj.	
<pre>modelObj = sbiomodel('cell');</pre>		<pre>biomodel('cell');</pre>

configsetObj = getconfigset(modelObj);

2 Configure the StopTimeType to approxWallTime.

set(configsetObj, 'StopTimeType', 'approxWallTime'); get(configsetObj, 'StopTimeType') ans = approxWallTime

See Also set, StatesToLog, StopTime, TimeUnits

### **Purpose** Specify label for SimBiology object

#### **Description**The Tag property specifies a label associated with a SimBiology object. Use this property to group objects and then use sbioselect to retrieve. For example, use the Tag property in reaction objects to group synthesis or degradation reactions. You can then retrieve all synthesis reactions using sbioselect. Similarly, for species objects you can enter and store classification information, for example, membrane protein, transcription factor, enzyme classifications, or whether a species is an independent variable. You can also enter the full form of the name of the species. This is useful when viewing the model in the Block Diagram Explorer. For example, the species object Name could be G6P for convenience, but in the Tag you should enter the full name, Glucose-6 phosphate. The graphical representation of the model in the Block Diagram Explorer (available in sbiodesktop) can be sorted by the Tag field, and this feature provides a method to view the full name.

### **Characteristics**

	Applies to	Objects: abstract kinetic law, kinetic law, model, parameter, reaction, rule, and species	
	Data type	char string	
	Data values	Any char string	
	Access	Read/write	
Examples	<pre>I Create a model object. modelObj = sbiomodel ('my_model');</pre>		
	<b>2</b> Add a reaction object and set the Tag property to 'Synthesis Reaction'.		
	reactionObj = addreaction (modelObj, 'a + b -> c + d') set (reactionObj, 'Tag', 'Synthesis Reaction')		
	<b>3</b> Verify the Tag a	assignment.	

get (reactionObj, 'Tag'); MATLAB returns: ans = 'Synthesis Reaction' addkineticlaw, addparameter, addreaction, addrule, addspecies,

See Also addkineticlaw, addparameter, addreaction, addrule, addspecies sbioabstractkineticlaw, sbiomodel, sbioroot

### Purpose Event trigger

# **Description** A Trigger is a condition that must become true for an event to be executed. You can a combination of relational and logical operators to build a trigger expression. Trigger can be a string, an expression, or a function handle that when evaluated returns a value of true or false. Triggers can access species, parameters, and compartments.

A trigger can contain the keyword 'time', to define an event that occurs at a specific time during the simulation.

For more information about how the SimBiology software handles events, see "How Events Are Evaluated" in the SimBiology User's Guide documentation. For examples of event functions, see "Specifying Event Triggers" in the SimBiology User's Guide documentation.

### **Characteristics**

	Applies to	Object: event	
	SimBiology type	String, function handle	
	SimBiology values	Specify MATLAB expression as string. Default is '' (None).	
	Access	Read/write	
Examples	<pre>1 Create a model object, and then add an event object. modelObj = sbmlimport('oscillator'); eventObj = addevent(modelObj, 'time&gt;= 5', 'OpC = 200'); 2 Set the Trigger property of the event object. set(eventObj, 'Trigger', '(time &gt;=5) &amp;&amp; (speciesA&lt;1000)');</pre>		
	<b>3</b> Get the Trigger p	roperty.	
	get(eventObj,	'Trigger')	

# Trigger

See Also Event object, EventFcns

Purpose	Show simulation time steps		
Description	The Time property shows the time points in a simulation.		
<b>Characteristics</b>	ics		
	Applies to	Object: SimData	
	Data type	double	
	Data values	Vector of doubles	
	Access	Read-only	
See Also	StopTime, StopTimeType		

# **TimeUnits**

Purpose	Show stop time units for simulation	
Description	The TimeUnits property shows units for the stop time for a simulation. The type of StopTime is specified in the property StopTimeType. Unit is in seconds.	
<b>Characteristics</b>		
	Applies to	Object: configset
	Data type	string
	Data values	Default value is second.
	Access	Read-only
See Also	StopTime, StopTimeType	

Purpose	Display top-level SimBiology object type		
Description	The Type property indicates a SimBiology object type. When you create a SimBiology object, the value of Type is automatically defined.		
	For example, when a Species object is created, the value of the Type property is automatically defined as 'species'.		
Characteristics	Applies to Objects: abstract kinetic law, configuration set, CompileOptions, kinetic law, model, parameter, reaction, root, rule, species, RuntimeOptions, and SolverOptions		
	Data type char string		
	Data values	abstract_kinetic_law, configset, compileoptions, kineticlaw, parameter, reaction, root, rule, runtimeoptions, sbiomodel, species, and solveroptions	
	Access	Read-only	
See Also	sbiomodel, sbiopara sbiospecies	ameter, sbioreaction, sbioroot, sbiorule,	

## **UnitConversion**

Purpose	Perform unit conversion	
Description	The UnitConversion property specifies whether to perform unit conversion for the model before simulation. It is a property of the CompileOptions object. CompileOptions holds the model's compile time options and is the object property of the configset object.	
<ul> <li>When UnitConversion is set to true, the SimBiology software constitution of the matching physical quantities to one consistent unit system in to resolve them. This conversion is in preparation for correct simule but species amounts are returned in the user-specified units.</li> <li>For example, consider a reaction a + b &gt; c. Using mass action kinetics the reaction rate is defined as a*b*k where k is the rate constant of the reaction. If you specify that initial amounts of a an are 0.01M and 0.005M respectively, then units of k are 1/(M*seco If you specify k with another equivalent unit definition, for example 1/((molecules/liter)*second), UnitConversion occurs after DimensionalAnalysis.</li> </ul>		quantities to one consistent unit system in order onversion is in preparation for correct simulation,
		te is defined as a*b*k where k is the rate a. If you specify that initial amounts of a and b respectively, then units of k are 1/(M*second). other equivalent unit definition, for example, o*second), UnitConversion occurs after
	Unit conversion requires dimensional analysis. If DimensionalAnalysis is off, and you turn UnitConversion on, then DimensionalAnalysis is turned on automatically. If UnitConversion is on and you turn off DimensionalAnalysis, then UnitConversion is turned off automatically.	
If UnitConversion fails, then you see an error when (sbiosimulate).		s, then you see an error when you simulate
	If UnitConversion is set to false, the simulation uses the given object values.	
Characteristics	Applies to	Object: CompileOptions (in configset object)

Data type

boolean

	Data values	true or false. Default value is false.
	Access	Read/write
Examples	_	w to retrieve and set unitconversion from the n the default configuration set in a model object.
	I Import a model.	
	modelObj = sbml	import('oscillator')
	SimBiology Mode	l - Oscillator
	_	0 : 0
		Settings - default (active)
	SolverOption AbsoluteTo RelativeTo	lerance: 1.000000e-006
	RuntimeOptio StatesToLo	
	CompileOptio	ns:

	UnitConversion: DimensionalAnalysis:	false true	
	<pre>3 Retrieve the CompileOptions object.     optionsObj = get(configsetObj,'CompileOptions')</pre>		
	Compile Settings:		
	UnitConversion: DimensionalAnalysis:	false true	
	<b>4</b> Assign a value of false to UnitConversion.		
	set(optionsObj,'UnitConve	ersion', true)	
See Also	get, getconfigset, sbiosimulate,	set	

**Description** Property to specify data that you want to associate with a SimBiology object. The object does not use this data directly, but you can access it using the function get or dot notation.

### **Characteristics**

Applies to	Objects: abstract kinetic law, configuration set, compartment, data, event, kinetic law, model, parameter, reaction, rule, species, or unit
Data type	Any
Data values	Any. Default is empty
Access	Read/write

See Also sbioabstractkineticlaw, sbiomodel, sbioparameter, sbioreaction, sbioroot, sbiorule, sbiospecies, sbiounit, sbiounitprefix

Purpose	Contain user-defined kinetic laws           Note         UserDefinedKineticLaws has been removed and produces an error. Use UserDefinedLibrary instead.		
Description	The UserDefinedKineticLaws property is a SimBiology root object property showing all user-defined abstract kinetic laws. Use the command sbiowhos -userdefined -kineticlaw to see the list of user-defined kinetic laws. You can use user-defined kinetic laws when you use the command addkineticlaw to create a kinetic law object for a reaction object. Refer to the kinetic law by name when you create the kinetic law object, for example:		
	<pre>kineticlawObj = addkineticlaw(reactionObj, 'my_kinetic_law');</pre>		
	You can add, modify, or delete UserDefinedKineticLaws. Create an abstract kinetic law with the command sbioabstractkineticlaw and add it to the user-defined kinetic law library with the command sbioaddtolibrary. sbioaddtolibrary also updates the UserDefinedKineticLaws property of the root object.		
	See "Abstract Kinetic Law" on page 6-49 for a definition and more information.		
<b>Characteristics</b>			
	Applies to	Object: root	
	Data type	char string	
	Data values	Valid kinetic laws	
	Access	Read/write	
See Also	AbstractKineticLaw object, UserDefinedLibrary	sbioaddtolibrary,	

### Purpose Library of user-defined components

# **Description** UserDefinedLibrary is a SimBiology root object property containing all user-defined components of unit, unit prefixes, and abstract kinetic laws that you define. You can add, modify, or delete components in the user-defined library. The UserDefinedLibrary property is an object that contains the following properties:

- Units Contains any user-defined units. You can specify units for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the user-defined units either by using the command sbiowhos -userdefined -unit, or by accessing the root object.
- UnitPrefixes Contains any user-defined unit prefixes. You can specify unit prefixes in combination with a valid unit for compartment capacity, species amounts and parameter values, to do dimensional analysis and unit conversion during simulation. You can display the user-defined unit prefixes either by using the command sbiowhos -userdefined -unitprefix, or by accessing the root object.
- KineticLaws Contains any user-defined unit abstract kinetic laws. Use the command sbiowhos -userdefined -kineticlaw to see the list of user-defined kinetic laws. You can use user-defined kinetic laws when you use the command addkineticlaw to create a kinetic law object for a reaction object. Refer to the kinetic law by name when you create the kinetic law object, for example, kineticlawObj
   addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');.

See "Abstract Kinetic Law" on page 6-49 for a definition and more information.

### **Characteristics**

Applies to	Object: root
Data type	object

Data values	Unit, unit prefix, and abstract kinetic la objects
Access	Read-only
Characteristics for U	IserDefinedLibrary properties:
• Units	
Applies to	UserDefinedLibrary property
Data type	Unit objects
Data values	Units
Access	Read/write
• UnitPrefixes	
Applies to	BuiltInLibrary property
Data type	Unit prefix objects
Data values	Unit prefixes
Access	Read/write
• KineticLaws	
Applies to	BuiltInLibrary property
Data type	Abstract kinetic law object
Data values	Kinetic laws

### Examples Example 1

This example uses the command sbiowhos to show the current list of user-defined components.

sbiowhos -userdefined -kineticlaw

```
sbiowhos -userdefined -unit
sbiowhos -userdefined -unitprefix
```

### Example 2

This example shows the current list of user-defined components by accessing the root object.

```
rootObj = sbioroot;
get(rootObj.UserDefinedLibrary, 'KineticLaws')
get(rootObj.UserDefinedLibrary, 'Units')
get(rootObj.UserDefinedLibrary, 'UnitPrefixes')
See Also BuiltInLibrary, sbioaddtolibrary, sbioremovefromlibrary
sbioroot, sbiounit, sbiounitprefix
```

**Purpose** Contain user-defined unit prefixes **Note** UserDefinedUnitPrefixes has been removed and produces an error. Use UserDefinedLibrary instead. **Description** The UserDefinedUnitPrefixes property is a SimBiology root object property showing all user-defined unit prefixes. You can specify units with prefixes for species amounts and parameter values to do dimensional analysis and unit conversion during simulation. The valid units and unit prefixes are either built in or user defined. Use the command sbiowhos -userdefined -unit to see the list of user-defined units. You can add, modify, or delete UserDefinedUnitPrefixes. You can define a unit prefix with the command sbioregisterunitprefix. which enables you to create the unit and add it to the user-defined unit prefixes library, and also add it to the UserDefinedUnitPrefixes property of the root object. **Characteristics** Applies to **Object:** root Data type char string Data values Valid unit prefixes

**See Also** sbioaddtolibrary, UserDefinedLibrary, UnitPrefix object

Access

Read/write

### Purpose Contain user-defined units

**Note** UserDefinedUnits has been removed and produces an error. Use UserDefinedLibrary instead.

**Description** The UserDefinedUnits property is a SimBiology root object property showing all user-defined units. You can specify units for species amounts and parameter values to do dimensional analysis and unit conversion during simulation. The valid units are either built in or user defined. Use the command sbiowhos -userdefined -unit to see the list of user-defined units.

You can add, modify, or delete UserDefinedUnits. You can define a unit with the command sbioregisterunit, which enables you to create the unit and add it to the user-defined units library, and also add it to the UserDefinedUnits property of the root object.

### **Characteristics**

Applies to	Object: root
SimBiology type	char string
SimBiology values	Valid units
SimBiology	Read/write

See Also sbioaddtolibrary, UserDefinedLibrary, Unit object

## Value

Purpose	Assign value to parameter object					
Description	The Value property is the value of the parameter object. The parameter object defines an assignment that can be used by the model object and/or the kinetic law object. Create parameters and assign Value using the method addparameter.					
Characteristics	Applies to Data type Data values Access	Object: parameter double Any double. Default value is 1.0. Read/write				
Examples	<pre>Assign a parameter with a value to the model object. 1 Create a model object, and then add a reaction object.     modelObj = sbiomodel ('my_model'); 2 Add a parameter to the model object (modelObj) with Value 0.5.     parameterObj1 = addparameter (modelObj, 'K1', 0.5) MATLAB returns:     SimBiology Parameter Array     Index: Name: Value: ValueUnits:     1 K1 0.5</pre>					
See Also	addparameter, sbioparameter					

### Purpose Parameter value units

**Description** The ValueUnits property indicates the unit definition of the parameter object Value property. ValueUnits can be one of the built-in units. To get a list of the built-in units, use the sbioshowunits function. If ValueUnits changes from one unit definition to another, the Value does not automatically convert to the new units. The sbioconvertunits function does this conversion.

You can add a parameter object to a model object or a kinetic law object.

### **Characteristics**

	Applies to	Obje	Object: parameter				
	Data type	char	r string				
	Data values	Unit	from units	library. Default is ' ' (empty).			
	Access	Read	d/write				
Examples	Assign a parameter with a value to the model object.						
	<b>1</b> Create a model object, and then add a reaction object.						
	<pre>modelObj = sbiomodel('my_model');</pre>						
	2 Add a parameter with Value 0.5, and assign it to the model object (modelObj). parameterObj1 = addparameter(modelObj, 'K1', 0.5, 'ValueUnits', '1/second') MATLAB returns: SimBiology Parameter Array						
	Index: 1	Name: K1	Value: 0.5	ValueUnits: 1/second			
See Also	addparameter, sk	pioconver	tunits,sbi	oparameter, sbioshowunits			

# ValueUnits

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