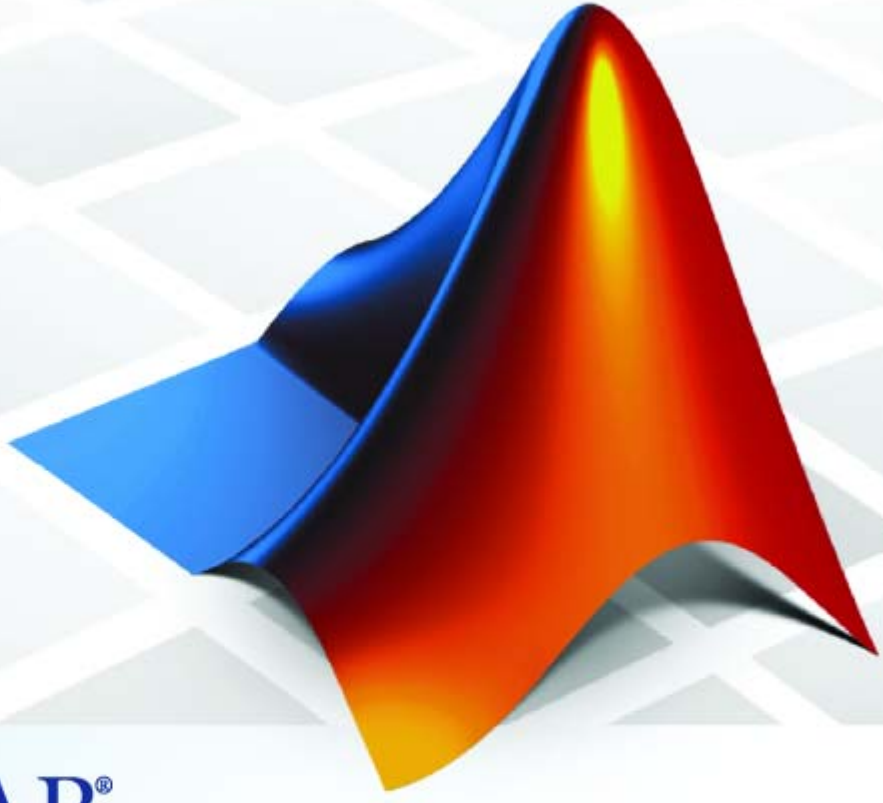
SimBiology 2
Reference



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SimBiology Reference

Revision History

September 2005	Online only	New for Version 1.0 (Release 14SP3+)
March 2006	Online only	Updated for Version 1.0.1 (Release 2006a)
May 2006	Online only	Updated for Version 2.0 (Release 2006a+)
September 2006	Online only	Updated for Version 2.0.1 (Release 2006b)
March 2007	Online only	Rereleased for Version 2.1.1 (Release 2007a)
September 2007	Online only	Rereleased for Version 2.1.2 (Release 2007b)
October 2007	Online only	Updated for Version 2.2 (Release 2007b+)

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Functions — By Category

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Saving and Opening Projects in MATLAB (p. 1-3)	Save and open projects in MATLAB®
Reading and Writing SBML Models (p. 1-4)	Export and Import SBML models
Constructing Objects (p. 1-5)	Create SimBiology™ objects
Working with 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

Saving and Opening Projects in MATLAB

`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

Reading and Writing SBML Models

`sbmlexport`	Export SimBiology model to SBML file
`sbmlimport`	Import SBML-formatted file

Constructing Objects

`sbioabstractkineticlaw`	Construct abstract kinetic law object
`sbioevent`	Construct event object
`sbiomodel`	Construct model object
`sbioparameter`	Construct parameter object
`sbioreaction`	Construct reaction object
`sbioroot`	Return SimBiology root object
`sbiorule`	Construct rule object
`sbiospecies`	Construct species object
`sbiovariant`	Construct variant object

Working with Units and Unit Prefixes

`sbioconvertunits`	Convert unit and unit value to new unit
`sbioregisterunitprefix`	Create user-defined unit prefix
`sbioshowunitprefixes`	Show unit prefixes in library
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`sbiounit`	Create user-defined unit
`sbiounitcalculator`	Convert value between units
`sbiounitprefix`	Create user-defined unit prefix

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Functions — Alphabetical List

sbioabstractkineticlaw

Purpose

Construct abstract kinetic law object

Syntax

```
abstkineticlawObj = sbioabstractkineticlaw('Name')
abstkineticlawObj = sbioabstractkineticlaw('Name',
   'Expression')
abstkineticlawObj = sbioabstractkineticlaw(...'PropertyName',
PropertyValue...)
```

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 *kineticlawObj*.
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. *abstkineticlawObj* = sbioabstractkineticlaw('*Name*') creates an abstract kinetic law object, with name *Name* and returns it to *abstkineticlawObj*.

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 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 *abstkineticlawObj* when constructing a kinetic law object with the method addkineticlaw, *abstkineticlawObj* 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').

abstkineticlawObj = sbioabstractkineticlaw('*Name*','*Expression*') constructs a SimBiology abstract kinetic law object, *abstkineticlawObj* with name, '*Name*' and with expression, '*Expression*' and returns it to *abstkineticlawObj*.

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).

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

Property Summary

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

`Tag`	Specify label for SimBiology object
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

Example

1 Create an abstract kinetic law.

```
abstkineticlawObj = sbioabstractkineticlaw('ex_mylaw1', '(k1*s)/(k2+k1+s)');
```

2 Assign the parameter and species variables in the expression.

```
set (abstkineticlawObj, 'SpeciesVariables', {'s'});
set (abstkineticlawObj, 'ParameterVariables', {'k1', 'k2'});
```

3 Add the new abstract kinetic law to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

SimBiology 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    ex_mylaw1    (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');
```

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 (abstkineticlawObj)
sbioaddtolibrary (unitObj)
sbioaddtolibrary (unitprefixObj)
```

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 *`kineticlawObj`*. For more information about creating a *`kineticlawObj`* see `sbioabstractkineticlaw`.
unitObj	Specify the user-defined unit to add to the library. For more information about creating *`unitObj`* see `sbiounit`.
unitprefixObj	Specify the user-defined unit-prefix to add to the library. For more information about creating *`unitprefixObj`* see `sbiounitprefix`.

Description

The function `sbioaddtolibrary` adds abstract kinetic laws, units, and unit-prefixes to the user-defined library.

`sbioaddtolibrary (`*`abstkineticlawObj`*`)` adds the abstract kinetic law object (`abstkineticlawObj`) to the user-defined library.

`sbioaddtolibrary (`*`unitObj`*`)` adds the user-defined unit (`unitObj`) to the user-defined library.

`sbioaddtolibrary (`*`unitprefixObj`*`)` adds the user-defined unit-prefix (`unitprefixObj`) to the user-defined library.

The `sbioaddtolibrary` function adds any abstract kinetic law, unit, or unit-prefix to the root object's `UserDefinedLibrary` property. These library components are available automatically in future MATLAB sessions.

Use the abstract kinetic law objects in the built-in and user-defined library to construct a kinetic law object with the method `addkineticlaw`.

To get a component of the built-in and user-defined libraries, use the commands `get(sbioroot, 'BuiltInLibrary')`, `(get(sbioroot, 'UserDefinedLibrary'))`.

To remove library component from the user-defined library, use the function `sbioremovefromlibrary`. You will not be able to remove an abstract kinetic law object being used by a kinetic law object.

Example

This example shows how to create an abstract kinetic law and add it to the user-defined library.

1 Create an abstract kinetic law.

```
abstkineticlawObj = sbioabstractkineticlaw('ex_mylaw1', '(k1*s)/(k2+k1+s)');
```

2 Assign the parameter and species variables in the expression.

```
set (abstkineticlawObj, 'SpeciesVariables', {'s'});
set (abstkineticlawObj, 'ParameterVariables', {'k1', 'k2'});
```

3 Add the new abstract kinetic law to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

SimBiology 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)
```

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');
```

Remember to specify the `SpeciesVariableNames` and the `ParameterVariableNames` in the `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

```
[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')
```

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`.
modelObj	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'` .
H	Cell array of strings containing the conserved moieties.
p	Prints the output to a cell array of strings.
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	Cell array containing the names of independent species in the model.

SD	Cell array containing the names of dependent species in the model.
L0	Link matrix relating SI and SD. The link matrix *L0* satisfies ND = L0*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 *modelObj*.
ND	Reduced stoichiometry matrices containing one row for each dependent species. The concatenated matrix [*NR*;*ND*] is a row-permuted version of the full stoichiometry matrix of *modelObj*.

Description

[*G*, *Sp*]= sbioconsmoiety(*modelObj*) calculates a complete set of linear conservation relations for the species in the SimBiology model object *modelObj*.

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', sbioconsmoiety 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'`, `sbioconsmoiety` 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 = sbioconsmoiety(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,L0,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

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.

```
 [g sp] = sbioconsmoiety(modelObj)

g =

     1     1     1


sp =

    'a'
    'b'
    'c'
```

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

```
sbioconvertunits(Obj, 'unit')
```

Description

`sbioconvertunits(Obj, 'unit')` converts the current `*Units` property on SimBiology object, *`Obj`* to the unit, *`unit`*. This function configures the `*Units` property to *`unit`* and updates the corresponding value property. For example `sbioconverunits` on a `speciesObj` updates the `InitialAmount` property value and the `InitialAmountUnits` property value.

`Obj` can be an array of SimBiology objects. *`Obj`* must be a SimBiology object that contains a unit property. The SimBiology objects that contain a unit property are compartment, parameter, and species objects. For example, if *`Obj`* is a species object with `InitialAmount` configured to `1` and `InitialAmountUnits` configured to `mole`, after the call to `sbioconvertunits` with *`unit`* specified as `molecule`, `speciesObj` `InitialAmount` is `6.0221e23` and `InitialAmountUnits` is `molecule`.

Example

Convert the units of the initial amount of glucose from `molecule` to `mole`.

1 Create the species `'glucose'` and assign an initial amount of `23` `molecule`.

At the command prompt type

```
speciesObj = sbiospecies ('glucose', 23, 'InitialAmountUnits', 'molecule')


SimBiology Species Array

Index: Compartment: Name: InitialAmount: InitialAmountUnits:
   1               glucose    23           molecule
```

2 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
```

InitialAmount value is changed.

```
get (speciesObj, 'InitialAmount')


ans =

  3.8192e-023
```

See Also

`sbioshowunits`

Purpose

Copy library to disk

Syntax

```
sbiocopylibrary ('kineticlaw','LibraryFileName')
sbiocopylibrary ('unit','LibraryFileName')
```

Description

`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.

`sbiocopylibrary ('unit','LibraryFileName')` copies all user-defined units and unit-prefixes to the file `LibraryFileName.sbulib`.

To get the abstract kinetic law objects in the built-in and user-defined libraries, use the commands `get(sbioroot, 'BuiltInKineticLaws')`, `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.

Example

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.

1 Create an abstract kinetic law.

```
abstkineticlawObj = sbioabstractkineticlaw('mylaw1', '(k1*s)/(k2+k1+s)');
```

2 Add the new abstract kinetic law to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

SimBiology 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 Copy the user-defined kinetic law library.

```
sbiocopylibrary ('kineticlaw','myLibFile')
```

4 Verify with `sbiowhos`.

```
sbiowhos -kineticlaw myLibFile
```

See Also

`sbioaddtolibrary`, `sbioabstractkineticlaw`, `sbioregisterunit`, `sbioregisterunitprefix`, `sbioremovefromlibrary`

Purpose

Open SimBiology modeling and simulation GUI

Syntax

```
sbiodesktop
sbiodesktop(modelObj)
```

Arguments

modelObj	Model 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 each model object in a separate model session.

Description

`sbiodesktop` opens the SimBiology GUI. The SimBiology GUI lets you do the following:

- Build a SimBiology model using reaction pathways and enter kinetic data for the reactions.
- Import or export SimBiology models to and from the MATLAB workspace or from a Systems Biology Markup Language (SBML) file.
- Modify an existing SimBiology model.
- Simulate a SimBiology model.
- View results from the simulation.
- Create and/or modify user-defined units and unit prefixes.
- Create and/or modify user-defined abstract kinetic law objects.

`sbiodesktop(modelObj)` opens the SimBiology GUI with a top-level SimBiology model object (*modelObj*). A top-level SimBiology model object has its property `Parent` set to the SimBiology root object.

Example

Create a SimBiology model in the MATLAB workspace, and then open the GUI with the model.

```
modelObj = sbiomodel('cell');
```

```
sbiodesktop(modelObj)
```

See Also

sbioroot

Purpose

Show results of ensemble run using 2-D or 3-D plots

Syntax

```
sbioensembleplot(simdataObj)
sbioensembleplot(simdataObj, Names)
sbioensembleplot(simdataObj, Names, Time)
FH = sbioensembleplot(simdataObj, Names)
FH = sbioensembleplot(simdataObj, Names, Time)
```

Arguments

simdataObj	*simdataObj* is an object that contains simulation data. You can generate a *simdataObj* object using the function sbioensemblerun. All elements of *simdataObj* must contain data for the same states in the same model.
Names	*Names* must be 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 *Time* is not an element of the time vectors in *simdataObj*, then the function resamples *simdataObj* as necessary using linear interpolation.
FH	Array of handles to figure windows.

Description

sbioensembleplot(*simdataObj*)shows a 3-D shaded plot of time-varying distribution of all logged states in the SimData array *simdataObj*. The sbioensemblerun function plots an approximate distribution created by fitting a normal distribution to the data at every time step.

sbioensembleplot(*simdataObj*, *Names*) plots the distribution for the data specified by *Names*.

`sbioensembleplot(simdataObj, Names, Time)` plots a 2-D histograms of the actual data of the ensemble distribution of the states specified by `Names` at the particular time point `Time`.

`FH = sbioensembleplot(simdataObj, Names)` returns a returns an array of handles `FH`, to the figure window for the 3-D distribution plot.

`FH = sbioensembleplot(simdataObj, Names, Time)` returns an array of handles `FH`, to the figure window for the 2-D histograms.

Examples

This example shows you 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.

   ```
   sbioloadproject('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 to reduce the size of the data generated.

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

   ```
   FH1 = sbioensembleplot(simdataObj, 'z', 1.0);
   ```

5. Create a 3-D shaded plot of both species.

   ```
   FH2 = sbioensembleplot(simdataObj, {'x','z'});
   ```

See Also

`sbioensemblerun`, `sbioensemblestats`, `sbiomodel`

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	*simdataObj* is an object that contains simulation data generated by `sbioensemblerun`. All elements of *simdataObj* must contain data for the same states in the same model.
modelObj	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`.
variantObj	Specify the variant object to apply to the model during the ensemble simulation. For more information about variant objects see `Variant object`.

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 you how to perform an ensemble run and generate a 2D 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);
```

Note 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 2D 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

```
[t,m] = sbioensemblestats(simDataObj)
[t,m,v] = sbioensemblestats(simDataObj)
[t,m,v,n] = sbioensemblestats(simDataObj)
```

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 *simDataObj* using `sbiogetnamedstate`.
simDataObj	*simDataObj* is a cell array of SimData objects, where each SimData object holds data for a separate simulation run. All elements of *simDataObj* must contain data for the same states in the same model. When the time vectors of the elements of *simDataObj* are not identical, *simDataObj* is first resampled onto a common time vector (see *interpolation* 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

`[t,m] = sbioensemblestats(simDataObj)` computes the time-dependent ensemble mean *m* of the ensemble data *simDataObj* obtained by running `sbioensemblerun`.

`[t,m,v] = sbioensemblestats(simDataObj)` computes the time-dependent ensemble mean *m* and variance *v* for the ensemble run data *simDataObj*.

`[t,m,v,n] = sbioensemblestats(simDataObj)` computes the time-dependent ensemble mean *m* and variance *v* for the ensemble run data *simDataObj*. Each column of *m* or *v* describes the ensemble mean or variance of some state as a function of time.

Examples

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

1 Load a SimBiology model `m1` from a SimBiology project file.

```
sbioloadproject('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`, `sbiomodel`, `sbiogetnamedstate`

sbioevent

Purpose

Construct event object

Syntax

```
eventObj = sbioevent(TriggerValue, EventFcnsValue)
eventObj = sbioevent(...'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 the"Property Summary" on page 2-29 table below.
PropertyValue	Property value. For more information on property values see the property reference for each property listed in the Property Summary.

Description

`eventObj = sbioevent(`*`TriggerValue`*`, `*`EventFcnsValue`*`)` creates a SimBiology event object, assigns a value (*`TriggerValue`*) for the property `Trigger`, assigns a value (*`EventFcnsValue`*) to the property `EventFcns`, and returns the 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.

The preferred way to work with events is to add an event to a SimBiology model with the `addevent` function.

For details on how events are handled during a simulation, see “Events” in the SimBiology User Guide.

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

Method Summary

copyobj (any object)	Copy SimBiology object and its children
display (any object)	Display summary of SimBiology 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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

Examples

1 Create an event object.

```
eventObj = sbioevent('time>= 5', 'OpC = 200');
```

2 Get a list of properties for the event object.

```
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'
              Type: 'event'
          UserData: []
```

See Also

Methods — `addevent`, `copyobj`

Objects — `Event object`

Purpose

Get model object that generated simulation data

Syntax

```
modelObj = sbiogetmodel(simDataObj)
```

Arguments

simDataObj	SimData object returned by the function `sbiosimulate` or by `sbioensemblerun`.
modelObj	Model object associated with the SimData object.

Description

`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.

If the SimBiology model used to generate the SimData object (*simDataObj*) is not currently loaded, *modelObj* is empty.

Example

Retrieve the model object that generated the SimData object.

1 Create a model object, simulate, and then return the results as a SimData object.

```
modelObj = sbmlimport('oscillator');
simDataObj = sbiosimulate(modelObj);
```

2 Get the model that generated the simulation results.

```
modelObj2 = sbiogetmodel(simDataObj)
SimBiology Model - Oscillator

Model Components:
  Models:           0
  Parameters:       0
  Reactions:        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

Note `sbiogetnamedstate` produces a warning and will be removed in a future version. Use `selectbyname` instead.

Syntax

```
[t,x]= sbiogetnamedstate(simDataObj)
[t,x]= sbiogetnamedstate(simDataObj,'Name')
[t,x, Name]= sbiogetnamedstate(...)
```

Description

`sbiogetnamedstate` returns state and time data from simulation results. `[t,x]= sbiogetnamedstate(simDataObj)` returns the time and state data associated with the simulation results (*`simDataObj`*) and returns to *`t`* and *`x`* respectively. *`simDataObj`* is a SimData object returned by the `sbiosimulate` function.

- *`t`* is a `n-by-1` vector of time samples labelling the rows of *`x`*.
- *`x`* is a `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 matrix from simulation results

Note `sbiogetsensmatrix` produces a warning and will be removed in a future version. Use `getsensmatrix` instead.

Syntax

```
[T,R,States,Inpfacs] = sbiogetsensmatrix(simDataObj)
[T,R,Outputs,Inpfacs] = sbiogetsensmatrix(imDataobj,
   OutNames, InpFacNames)
```

Arguments

T	Column vector of length `m` specifying time points for the sensitivity data in *R*.
R	`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 *R*. `R(:,i,j)` is the time course for the sensitivity of state *Outputs*{*i*} to the input factor *Inpfacs*{*j*}. When *simdataObj* contains more than one element, the output arguments are cell arrays in which each cell contains data for the corresponding element of *simdataObj*.
Inpfacs	Contains names of the input factors that label the third dimension of *R*. `R(:,i,j)` is the time course for the sensitivity of states *Outputs*{*i*} to the input factor *Inpfacs*{*j*}.
simDataObj	SimData object returned by `sbiosimulate`. Contains sensitivity data when sensitivity analysis is enabled.

OutNames	Specify outputs to get sensitivity data from *simDataObj*. Can be an empty array, or a single name, or a cell array of names. When empty array is specified, returns the sensitivity data on all species states contained in *simDataObj*.
InpFacNames	Specify input factors to get sensitivity data from *simDataObj*. Can be an empty array, or a single name, or a cell array of names. When empty array is specified, returns the sensitivity data for all input factors contained in *simDataObj*.

Description

`[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*.

The sensitivity data that is logged in *simDataObj* is set at simulation time by the active configuration set that is used during the simulation. Note that the sensitivity data *R* returned by `sbiogetsensmatrix` may be normalized, as specified at simulation time.

`[T,R,Outputs,Inpfacs] = sbiogetsensmatrix(imDataobj, OutNames, InpFacNames)` gets sensitivity data for the outputs specified by *OutNames* and the input factors specified by *InpFacNames*.

See Also

`getsensmatrix` `sbiogetnamedstate`, `sbiohelp`, `sbiosimulate`

sbiohelp

Purpose

Help for SimBiology functions

Syntax

```
sbiohelp('FunctionName')
h = sbiohelp ('FunctionName')
```

Description

`sbiohelp('FunctionName')` displays information for a SimBiology function (*`FunctionName`*).

`h = sbiohelp ('FunctionName')` returns the help for the SimBiology function *`FunctionName`* to `h`.

General information on SimBiology can be returned by specifying *`FunctionName`* as 'sbio'. General information about a SimBiology object can be returned by specifying *`FunctionName`* as one of the following: `'AbstractKineticLaw'`, `'KineticLaw'`, `'Model'`, `'Parameter'`, `'Reaction'`, `'Root'`, `'Rule'`, `'Species'`, `'Configset'`, `'CompileOptions'`, `'ExplicitTauSolverOptions'`, `'ImplicitTauSolverOptions'`, `'ODESolverOptions'`, `'RuntimeOptions'`, or `'SSASolverOptions'`.

Examples

```
sbiohelp('addreaction')
sbiohelp addreaction
sbiohelp reaction
sbiohelp('sbioshowunits')
```

See Also

MATLAB function `help`

Purpose

SimBiology last error message

Syntax

```
sbiolasterror
diagstruct = sbiolasterror
sbiolasterror([])
sbiolasterror(diagstruct)
```

Arguments

diagstruct	The diagnostic structure holding `Type`, `Message ID` and `Message` for the errors.

Description

`sbiolasterror` or *`diagstruct`* `= sbiolasterror` return a SimBiology diagnostic structure array containing the last error(s) generated by SimBiology. The fields of the diagnostic structure are:

Type	`'error'`
MessageID	The message ID for the error, (for example, `'SimBiology:ConfigSetNameClash'`)
Message	Error message

`sbiolasterror([])` resets the SimBiology last error so that it will return an empty array until the next SimBiology error is encountered.

`sbiolasterror(`*`diagstruct`*`)` will set the SimBiology last error(s) to those specified in the diagnostic structure (*`diagstruct`*).

Examples

The following example shows you how to use `verify` and `sbiolasterror`.

1 Import a model.

```
a = sbmlimport('radiodecay.xml')

SimBiology Model - RadioactiveDecay

 Model Components:
```

```
  Models:           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

??? Error using ==> simbio\private\odebuilder>buildPatternSubStrings
The object y does not resolve on reaction with expression 'x*y'.

Error in ==> sbiogate at 22
 feval(varargin{:});

??? --> Error reported from Expression Validation :
The object 'y' in reaction 'Reaction1' does not resolve to any in-scope species
                                                                    or parameters.
--> Error reported from Dimensional Analysis :
Could not resolve species, parameter or model object 'y' during dimensional analysis.
--> Error reported from ODE Compilation:
Error using ==> simbio\private\odebuilder>buildPatternSubStrings
The object y does not resolve on reaction with expression 'x*y'.
```

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

Purpose

SimBiology last warning message

Syntax

```
sbiolastwarning
diagstruct = sbiolastwarning
sbiolastwarning([])
sbiolastwarning(diagstruct)
```

Arguments

diagstruct	The diagnostic structure holding `Type`, `Message ID` and `Message` for the warnings.

Description

`sbiolastwarning` or *`diagstruct`* `= sbiolastwarning` return a SimBiology diagnostic structure array containing the last warnings generated by SimBiology. The fields of the diagnostic structure are:

Type	`'warning'`
MessageID	The message ID for the warning (for example, `'SimBiology:DANotPerformedReactionRate'`)
Message	The warning message

`sbiolastwarning([])` resets the SimBiology last warning so that it will return an empty array until the next SimBiology warning is encountered.

`sbiolastwarning(`*`diagstruct`*`)` will set the SimBiology last warnings to those specified in the diagnostic structure (*`diagstruct`*).

See Also

`sbiolasterror`, `verify`

sbioloadproject

Purpose

Load project from file

Syntax

```
sbioloadproject('projFilename')
sbioloadproject ('projFilename','variableName')
sbioloadproject projFilename variableName variableName2
```

Description

`sbioloadproject('projFilename')` loads a SimBiology project from a project file (*projFilename*). If no extension is specified SimBiology assumes a default extension of `.sbproj`. Alternatively, the command syntax is `sbioloadproject projFilename`

You can also use the function syntax as follows:

`sbioloadproject ('projFilename','variableName')` loads only the variable *variableName* from the project file.

`sbioloadproject projFilename variableName variableName2` loads the specified variables, from the project. The contents of the project file can be displayed by using the `sbiowhos` command.

See Also

`sbiosaveproject`, `sbiowhos`, `sbioaddtolibrary`, `sbioremovefromlibrary`

Purpose

Construct model object

Syntax

```
modelObj = sbiomodel('NameValue')
modelObj = sbiomodel(...'PropertyName', PropertyValue...)
```

Arguments

NameValue	Required property to specify a unique name for a `model` object. Enter a character string.
PropertyName	Property name for a `Model` object from the Property Summary table below.
PropertyValue	Property value. Valid value for the specified property.

Description

`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`.

`modelObj = sbiomodel(...'PropertyName', PropertyValue...)` defines optional properties. The property name and 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).

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

Property Summary

`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
`Tag`	Specify label for SimBiology object
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

Examples

1 Create a SimBiology model object.

```
modelObj = sbiomodel('cell', 'Tag', 'mymodel');
```

2 List all `modelObj` properties and the current values.

```
get(modelObj)
```

MATLAB returns

```
      Annotation: ''
          Models: [0x1 double]
```

```
          Name: 'cell'
         Notes: ''
    Parameters: [0x1 double]
        Parent: [1x1 SimBiology.Root]
       Species: [0x1 double]
     Reactions: [0x1 double]
         Rules: [0x1 double]
           Tag: 'mymodel'
          Type: 'sbiomodel'
      UserData: []
```

3 Display summary of `modelObj` contents.

```
modelObj

  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`, `sbioroot`, `copyobj`, `sbiosimulate`

MATLAB functions `get`, `set`

Purpose

Perform parameter estimation

Syntax

```
[k, result]= sbioparamestim(modelObj, tspan, xtarget,
   species_array, parameter_array))
[...]= sbioparamestim(..., species_array, parameter_array,
   k0)
[...]= sbioparamestim(..., species_array, parameter_array,
   k0, method)
```

Arguments

k	Vector of estimated parameter values.
result	`struct` with fields that provide information about the progress of optimization.
tspan	`n-by-1` vector representing the time span of the target data *xtarget*.
xtarget	`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 only be species varying with time. You cannot use time varying (non-constant) parameters. The number of rows of *xtarget* must be the same as the number of rows of *tspan*.

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 species correctly. `sbioparamestim` assumes that 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 *parameter_array* is 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*, SimBiology 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`.

k0

Array of doubles that holds initial values of parameters to be estimated. The length of *k0* is same as that of *parameter_array*. When you specify *k0*, `sbioparamestim` ignores any initial values specified in active variants attached to the model. If left unspecified, SimBiology takes initial values for parameters from the model(*modelObj*) or if there are active variants `sbioparamestim` uses any initial values specified in the active variants. See `Variant object` for more information about variants.

method

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`.

SimBiology 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, use 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`, species specified in `sp_array`, using different algorithms. This example uses the data from "Example 1" on page 2-50.

```
[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 2-50.

```
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 function `gaoptimset`, `psoptimset`

Purpose

Construct parameter object

Syntax

```
parameterObj = sbioparameter(Obj, NameValue)
parameterObj = sbioparameter(Obj, NameValue, ValueValue)
parameterObj = sbioparameter(...'PropertyName', PropertyValue...)
```

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

`parameterObj = sbioparameter(Obj, NameValue)` constructs a SimBiology parameter object, enters a value (*NameValue*) for the required property `Name`, and returns the object (`parameterObj`).

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

Property Summary

`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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object
`Value`	Assign value to parameter object
`ValueUnits`	Parameter value units

Examples

1 Construct a parameter object.

```
parameterObj = sbioparameter('kappa', 1);
% View the help for the parameter object's Value property.
help(parameterObj, 'Value')
```

2 View parameter object properties.

```
get(parameterObj)
```

MATLAB returns

```
          Annotation: ''
      ConstantValue: 1
               Name: 'kappa'
              Notes: ''
             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	SimBiology data object
fcnHandleValue	Function handle
xArgsValue	Cell array with the names of the states
yArgsValue	Cell array with the names of the states

Description

`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 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, YArgs
```

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 you 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`

Purpose

Construct reaction object

Syntax

```
reactionObj = sbioreaction('ReactionValue')
reactionObj = sbioreaction('ReactantsValue',
   'ProductsValue')
reactionObj = sbioreaction('ReactantsValue',
   RStoichCofficients, 'ProductsValue', PStoichCofficients)
reactionObj = sbioreaction(...'PropertyName', PropertyValue...)
```

Arguments

ReactionValue	Specify the reaction equation. Enter a character string. A hyphen preceded by a space and followed by a right angle bracket (`->`) indicate reactants going forward to products. A hyphen with left and right angle brackets (`<->`) indicate a reversible reaction. Coefficients before reactant or product names must be followed by a space. Examples `'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 *ReactantsValue*.
PStoichCofficients	Stoichiometric coefficients for products, length of array equal to length of *ProductsValue*.

Description

reactionObj = sbioreaction('*ReactionValue*') creates a SimBiology reaction object, assigns a value (ReactionValue) to the property Reaction, and returns the reaction object (*reactionObj*).

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.

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.

reactionObj = sbioreaction('*ReactantsValue*', *RStoichCofficients*, '*ProductsValue*', *PStoichCofficients*) adds stoichiometric coefficients (*RStoichCofficients*) for reactant species, and stoichiometric coefficients (PStoichCofficients) for product species, to the property Stoichiometry. The length of Reactants and RCofficients must be equal, and the length of Products and PCofficients must be equal.

reactionObj = sbioreaction(...'*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 additional reactionObj properties with the get command. Modify additional reactionObj 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, SimBiology 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

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
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants

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
`Tag`	Specify label for SimBiology object
`Type`	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: [0x1 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

Note `sbioregisterunit` produces a warning and will be removed in a future version. Use `sbiounit`, followed by `sbioaddtolibrary` instead.

Syntax

```
sbioregisterunit('Name', 'Composition', Multiplier)
sbioregisterunit('Name', 'Composition', Multiplier, Offset)
```

Description

`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.

`sbioregisterunit('Name', 'Composition', Multiplier, Offset)` creates a unit with the specified offset. You can list available units with the `sbioshowunits` function.

- *`Name`* is the name of the user-defined unit. *`Name`* must begin with characters and can contain characters, underscores or numbers. *`Name`* 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 SimBiology uses to define all unit quantity equations. Derived units are defined using base units or mixtures of base and derived units.
- *`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 `1 mole` is `6.0221e23*molecule`. The *`Multiplier`* is `6.0221e23`.
- *`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`.

See Also

sbioaddtolibrary, sbioremovefromlibrary, sbioshowunits, sbiounit

Purpose

Create user-defined unit prefix

Note `sbioregisterunitprefix` produces a warning and will be removed in a future version. Use `sbiounitprefix` followed by `sbioaddtolibrary` instead.

Syntax

```
sbioregisterunitprefix('NameValue', Exponent)
```

Description

`sbioregisterunitprefix('NameValue', Exponent)` creates a unit prefix with the name *`NameValue`* 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.

- *`NameValue`* 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).
- *`Exponent`* shows the value of `10^Exponent`that defines the relationship of the unit *`Name`* 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')`, `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

Shows you how to remove an abstract kinetic law from the user-defined library.

1. Create an abstract kinetic law.

```
abstkineticlawObj = sbioabstractkineticlaw('mylaw1', '(k1*s)/(k2+k1+s)');
```

2. Add the new abstract kinetic law to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

`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` delete 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

Shows you the difference between `sbioreset` and `clear all`.

1 Import a model into the workspace.

```
modelObj = sbmlimport('oscillator');
```

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:                          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
```

2 The command `clear all` clears the workspace, but the `modelObj` still exists on the `rootObj`.

```
clear all

rootObj


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 The command `sbioreset` deletes 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

```
rootObj = sbioroot
modelObj = sbioroot('modelName')
```

Arguments

rootObj	Return `sbioroot` to this object.
modelObj	Return the model with name *modelName* to this object.
modelName	Specify the name of the model that is on the root object.

Description

rootObj `= 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.

modelObj `= sbioroot('modelName')` returns the SimBiology model with name, `modelName` to `modelObj`. A SimBiology model object has its `Parent` property set to the SimBiology root object.

The units define the set of built-in units and user-defined units. See `Unit object` for more information.

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`.

Method Summary

copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
reset (root)	Delete all model objects from root object

Property Summary

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

Examples

1 Get all SimBiology model objects contained by the root.

```
rootObj = sbioroot;
allmodels = get(rootObj, 'Models');
```

2 Get the model with name `cell`.

```
modelObj = sbioroot('cell');
```

See Also

`addkineticlaw`, `sbiomodel`, `sbioreset`

sbiorule

Purpose

Construct rule object

Syntax

```
ruleObj = sbiorule('RuleValue')
ruleObj = sbiorule(RuleValue, 'RuleTypeValue')
ruleObj = sbiorule(...'PropertyName', PropertyValue...)
```

Arguments

RuleValue	Enter a character string within quotes. 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.

ruleObj = `sbiorule('`*RuleValue*`')`creates a rule object, assigns a value (*RuleValue*) to the property `Rule`, assigns the value `'algebraic'` to the property `RuleType`, and assigns the root object to the property `Parent`.

To use `ruleObj` in a simulation, `ruleObj` must be added to a model object with the function `copyobj`. Note that a rule can also be added to a SimBiology model with the `addrule` function. A model object is constructed with the function `sbiomodel`.

ruleObj = `sbiorule(`*RuleValue*`, '`*RuleTypeValue*`')` in addition to the above, this syntax enables you to specify `RuleType`.

`ruleObj = sbiorule(...'`*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 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

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

Examples

Example 1

Construct a rule object and copy 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` *`projFilename`* saves all models in the SimBiology root object to the binary SimBiology project file named *`projFilename`*`.sbproj`. The project can be loaded with `sbioloadproject`. SimBiology returns an error if *`projFilename`*`.sbproj` is not writable.

`sbiosaveproject` creates the binary SimBiology project file named `simbiology.sbproj`. SimBiology returns an error if this is not writable.

`sbiosaveproject` *`projFilename variableName`* saves only *`variableName`*. *`variableName`* can be a SimBiology model or any MATLAB variable.

`sbiosaveproject` *`projFilename variableName1 variableName2 ...`* 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 *`fileName`* and you want to store MATLAB variables *`variableName1`* and *`variableName2`*, type `sbiosaveproject(`*`fileName`*`, '`*`variableName1`*`', '`*`variableName2`*`')` at the command line.

Examples

1 Import an SBML file and simulate (default configset object is used).

```
modelObj = sbmlimport ('oscillator.xml');
timeseriesObj = sbiosimulate(modelObj);
```

2 Save the model and the simulation results to a project.

```
sbiosaveproject myprojectfile modelObj timeseriesObj
```

See Also

`sbioloadproject`, `sbiowhos`, `sbioaddtolibrary`, `sbioremovefromlibrary`

Purpose

Search for objects with specified constraints

Syntax

```
Out = sbioselect('PropertyName', PropertyValue)
Out = sbioselect('Where', 'PropertyName', 'Condition',
   PropertyValue)
Out = sbioselect(Obj, 'PropertyName', PropertyValue)
Out = sbioselect(Obj, 'Type', 'TypeValue', 'PropertyName',
   PropertyValue)
Out = sbioselect(Obj, 'Where', 'PropertyName' , 'Condition',
   PropertyValue)
Out = sbioselect(Obj, 'Where', 'PropertyName1', 'Condition1',
   PropertyValue1, 'Where', 'PropertyName2', 'Condition2',
   PropertyValue2,...)
Out = sbioselect(Obj, 'Depth', DepthValue,...)
```

Arguments

Out	Object or array of objects returned by the `sbioselect` function. *Out* might contain a mixture of object types (for example, species and parameters), depending on the selection you specify .If *PropertyValue* is a cell array, then the function returns all objects with the property '*PropertyName*' that matches any element of *PropertyValue*.
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 *PropertyValue* to include in 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 2-77 for a list of conditions.
DepthValue	Specify the depth number to search. Valid numbers are positive integer values and `inf`. If *DepthValue* is `inf`, `sbioselect` searches *Obj* and all of its children. If *DepthValue* is `1`, sbioselect only searches *Obj* and not its children. By default, *DepthValue* is `inf`.

Description

`sbioselect` searches for objects with specified constraints.

Out = `sbioselect('`*PropertyName*`',` *PropertyValue*`)` searches the root object (including all model objects contained by the root object) and returns the objects with the property name (*PropertyName*) and property value (*PropertyValue*) contained by the root object.

Out = `sbioselect('Where', '`*PropertyName*`', '`*Condition*`',` *PropertyValue*`)` searches the root object and finds objects that have a property name (*PropertyName*) and value (*PropertyValue*) that matches the condition (*Condition*).

Out = `sbioselect(`*Obj*`, '`*PropertyName*`',` *PropertyValue*`)` returns the objects with the property name (*PropertyName*) and property value (*PropertyValue*) found in any object (*Obj*).

Out = `sbioselect(`*Obj*`, 'Type', '`*TypeValue*`', '`*PropertyName*`',` *PropertyValue*`)` finds the objects of type (`TypeValue`), with the property name (*PropertyName*) and property value (*PropertyValue*) found in any object (*Obj*). *TypeValue* is the type of SimBiology object to be included in the selection, for example, `species`, `reaction`, or `kineticlaw`.

Out = `sbioselect(`*Obj*`, 'Where', '`*PropertyName*`' , '`*Condition*`',` *PropertyValue*`)` finds objects that have a property name (*PropertyName*) and value (*PropertyValue*) that matches the condition (*Condition*).

If you search for a string property value without specifying a condition, you must use the same format as `get` returns. For example, if `get` returns the `Name` as `'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 below:
	
	`parameterObj = sbioselect (modelObj,...`
	`'Value', 0.5)`
	
	Search in the model object (`modelObj`), and return parameter objects that have `ConstantValue false` (non-constant 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.
	
	`speciesObj = sbioselect (modelObj, ...`
	`'Where', 'InitialAmount', '>', 50)`
	
	Search in the model object (`modelObj`), and return species objects that have an initial amount (`InitialAmount`) less than or equal to 50.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Where', 'InitialAmount', '<=', 50)`

`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.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Where', 'InitialAmount',...`
	`'~between', [200 300])`

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

Conditions for String Properties	Example Syntax

`==`	Search in the model object (`modelObj`), and return species objects that have the name `'Glucose'`.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Type', 'species', 'Where',...`
	`'Name', '==', 'Glucose')`

`~=`	Search in the model object (`modelObj`), and return species objects that do not have the name `'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 do not have the name `'Glucose'`, ignoring case.
	
	`speciesObj = sbioselect (modelObj,...`
	`'Type', 'species', 'Where',...`
	`'Name', '~=i', 'glucose')`

Conditions for String Properties	Example Syntax

`regexp`. Supports expressions supported by the functions `regexp` and `regexpi`.	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).

`regexpi`	Same as `regexp`; in addition, this is case insensitive.

`~regexp`	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')`

`~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'`	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))`

`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.

```
modelObj.Species(2).UserData = {'a' 'b'};
Obj = sbioselect(modelObj,'UserData',{{'a' 'b'}})

SimBiology Species Array

Index:    Compartment:    Name:    InitialAmount:  InitialAmountUnit
1         unnamed         pB       0
```

See Also

`regexp`

Purpose

Show unit prefixes in library

Syntax

```
UnitPrefixObjs = sbioshowunitprefixes
[Name, Multiplier] = sbioshowunitprefixes
[Name, Multiplier, Builtin] = sbioshowunitprefixes
[Name, Multiplier, Builtin] = sbioshowunitprefixes('Name')
```

Arguments

unitPrefixObjs	Vector of unit prefix objects from the `BuiltInLibrary` and `UserDefinedLibrary` properties of the `Root object`.
Name	*Name* is the name of the built-in or user-defined unit prefix. Built-in prefixes are defined based on the International System of Units (SI).
Multiplier	*Multiplier* shows the value of `10^Exponent` that defines the relationship of the unit prefix *Name* to the base unit. For example the multiplier in `picomole` is `10e-12`.
Builtin	*Builtin* is an array of logical values. If *Builtin* is true for a unit prefix, the unit prefix is built-in. If *Builtin* is false for a unit prefix, the unit prefix is user-defined.

Description

`sbioshowunitprefixes` returns information about unit prefixes in the SimBiology library.

UnitPrefixObjs = `sbioshowunitprefixes` returns the unit prefixes in the library as a vector of unit prefix objects in *UnitPrefixObjs*.

[*Name, Multiplier*] = `sbioshowunitprefixes` returns the multiplier for each prefix in *Name* to *Multiplier* 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*.

`[Name, Multiplier, Builtin] = sbioshowunitprefixes('Name')` returns the name, multiplier, and built-in status for the unit prefix with name *Name*. *Name* can be a cell array of strings.

Examples

```
[name, multiplier] = sbioshowunitprefixes;
[name, multiplier] = sbioshowunitprefixes('nano');
```

See Also

`sbiounitprefix`, `sbioshowunits`, `sbioconvertunits`

Purpose

Show units in library

Syntax

```
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')
```

Arguments

unitObjs	Vector of unit objects from the `BuiltInLibrary` and `UserDefinedLibrary` properties of the `Root object`.
Name	*Name* is the name of the built-in or user-defined unit.
Composition	*Composition* shows the combination of base and derived units that defines the unit *Name*. For example `molarity` is `mole/liter`.
Multiplier	*Multiplier* is the numerical value that defines the relationship between the unit *Name* and the base or derived unit as a product of the *Multiplier* and the base unit or derived unit. For example `1 mole` is `6.0221e23*molecule`. The *Multiplier* is `6.0221e23`.

Offset	*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`.
Builtin	*Builtin* is an array of logical values. If *Builtin* is true for a unit, the unit is built-in. If *Builtin* is false for a unit, the unit is user-defined.

Description

unitObjs = `sbioshowunits` returns the units in the library to *unitObjs* as a vector of unit objects.

[*Name, Composition*] = `sbioshowunits` returns the composition for each unit in *Name* to *Composition* as a cell array of strings.

[*Name, Composition, Multiplier*] = `sbioshowunits` returns the multiplier for the unit with name *Name* to *Multiplier*.

[*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*.

[*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

```
[name, composition] = sbioshowunits;
[name, composition] = sbioshowunits('molecule');
```

See Also

`sbiounit`, `sbioshowunitprefixes`, `sbioconvertunits`

Purpose

Simulate model object

Syntax

```
[t,x,names] = sbiosimulate(modelObj)
simDataObj = sbiosimulate(modelObj)
... = sbiosimulate(modelObj, configsetObj)
... = sbiosimulate(modelObj, variantObj)
... = sbiosimulate(modelObj, configsetObj, variantObj)
```

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	*simdataObj* is 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 *simdataObj* through *simdataObj* properties. See `SimData object` for more information.

Input Arguments

modelObj	Model object to be simulated.
configsetObj	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

`[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 2-89.

simDataObj `= sbiosimulate(`*modelObj*`)` simulates the Simbiology model object (*modelObj*) and returns the results to a SimData object.

`...  = 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*).

`...  = sbiosimulate(`*modelObj*`,` *configsetObj*`,` *variantObj*`)` simulates a model object, (*modelObj*), using the configuration set object *configsetObj* and the variant object or array of variant objects (*variantObj*).

Property Summary

Configuration set 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
`Type`	Display top-level SimBiology object type

Examples

The following examples show you how to change solver settings.

Example 1

Create a SimBiology model from an SBML file, simulate the model using a solver other than the default solver (default is `ode15s`), and view the results.

1 Read the file for the`oscillator` model.

```
modelObj = sbmlimport('oscillator.xml');
```

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 `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 `modelObj`.

```
simDataObj = sbiosimulate(modelObj);
```

3 Plot the results of the simulation.

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

See Also

SimBiology object constructor `sbiomodel`, model object method `addconfigset`

sbiospecies

Purpose

Construct species object

Syntax

```
speciesObj = sbiospecies('NameValue')
speciesObj = sbiospecies('NameValue'),InitialAmountValue)
speciesObj = sbiospecies(...'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`.
IntialAmountValue	Initial amount value for the species object. Enter `double`. Positive real number, default = 0.

Description

speciesObj = sbiospecies('*NameValue*') constructs a `SimBiology.Species` object, enters a value (*NameValue*) for the property `Name`, and returns the object (`speciesObj`).

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

Species are entities that take part in reactions. A species object represents these entities. There are reserved characters you cannot use in species object name (*NameValue*)

In order for a species object to be used in a simulation, the `species` object must be added to a 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.

SimBiology automatically updates species names for reactions that use MassAction kinetic law. See Name for more information about specifying species names.

Method Summary

Methods for species objects.

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

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
`Tag`	Specify label for SimBiology object
`Type`	Display top-level SimBiology 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 with name `H2O` and initial amount 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: ''
                Type: 'species'
            UserData: []
```

Example 2

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

1. Create two species objects with the names `glucose_6_phosphate` and `glucose_6_phosphate_dehydrogenase`.

```
speciesObj1 = sbiospecies ('glucose_6_phosphate');
speciesObj2 = sbiospecies ('glucose_6_phosphate_dehydrogenase');
```

2. Set initial amount of `glucose_6_phosphate` to `100` and verify.

```
set(speciesObj1, 'InitialAmount', 100);
get(speciesObj1, 'InitialAmount')
```

MATLAB returns

```
ans =

   100
```

See Also

SimBiology method `addspecies`

MATLAB functions `get` and `set`

sbiosubplot

Purpose

Plot simulation results in subplots

Syntax

```
sbiosubplot(simDataObj)
sbiosubplot(simDataObj, fcnHandleValue, xArgsValue,
   yArgsValue)
sbiosubplot(simDataObj, fcnHandleValue, xArgsValue,
   yArgsValue, showLegendValue)
```

Arguments

simDataObj	SimBiology data object
fcnHandleValue	Function handle
xArgsValue	Cell array with the names of the states
yArgsValue	Cell array with the names of the states
showLegendValue	Boolean (default is false)

Description

`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 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 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*. *showLegendValue* indicates if a legend is shown in the plot. *showLegendValue* can be either true or false. By default, *showLegendValue* is false.

Examples

This example shows you 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');
        sbiosubplot(simDataObj);
```

See Also

sbioplot

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 — *NameValue* is the name of the user-defined unit. *NameValue* must begin with characters and can contain characters, underscores or numbers. *NameValue* can be any valid MATLAB variable name.

CompositionValue — *CompositionValue* shows the combination of base and derived units that defines the unit *NameValue*. 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 — *MultiplierValue* is the numerical value that defines the relationship between the user-defined unit *NameValue* and the base unit as a product of the *MultiplierValue* and the base unit. For example `1 mole` is `6.0221e23*molecule`. The *MultiplierValue* is `6.0221e23`.

OffsetValue — *OffsetValue* is the numerical value by which the unit composition is modified. For example `Celsius = (5/9)*( Fahrenheit-32);` `Fahrenheit` is `Composition`; *MultiplierValue* is `5/9` and *OffsetValue* is `32`.

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

unitObject = sbiounit('*NameValue*') constructs a SimBiology unit object with name, *NameValue*. Valid names must begin with a letter, and be followed by letters, underscores, or numbers.

unitObject = sbiounit('*NameValue*', '*CompositionValue*') allows you to specify the name and the composition of the unit.

unitObject = sbiounit('*NameValue*','*CompositionValue*',*MultiplierValue*) creates a unit with the name *NameValue* where the unit is defined as MultiplierValue*CompositionValue.

unitObject = sbiounit('*NameValue*','*CompositionValue*',*MultiplierValue*,*OffsetValue*) creates a unit with the specified offset.

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).

In order to use *unitObject*, you must add it to the user-defined library with the sbioaddtolibrary function. To get the unit object into the user-defined library, use the following command:

```
sbioaddtolibrary(unitObject);
```

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
```

```
Index:  Name:            Composition:          Multiplier:     Offset:

1       firstconstant     1/second             1.000000        0.000000

2       secondconstant    1/molarity*second    1.000000        0.000000
```

See Also

sbioshowunits, sbiounitprefix, sbioaddtolibrary, sbiowhos

sbiounitcalculator

Purpose

Convert value between units

Syntax

```
result = sbiounitcalculator('fromUnits', 'toUnits', Value)
```

Description

`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`*.

Example

```
result = sbiounitcalculator('mile/hour','meter/second',1)
```

See Also

`sbioshowunits`

Purpose

Create user-defined unit prefix

Syntax

```
unitprefixObject = sbiounitprefix('NameValue')
unitprefixObject = sbiounitprefix('NameValue',
   'ExponentValue')
unitprefixObject = sbiounitprefix('NameValue',
   ...'PropertyName', PropertyValue ...)
```

Arguments

NameValue	*NameValue* is the name of the user-defined unit prefix. *NameValue* must begin with characters and can contain characters, underscores or numbers. *NameValue* can be any valid MATLAB variable name.
ExponentValue	*ExponentValue* shows the value of `10^Exponent` that defines the relationship of the unit *Name* 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

unitprefixObject = sbiounitprefix('*NameValue*') constructs a SimBiology unit prefix object with name, *NameValue*. Valid names must begin with a letter, and be followed by letters, underscores, or numbers.

unitprefixObject = sbiounitprefix('*NameValue*', '*ExponentValue*') creates a unit prefix object with a multiplicative factor of 10^'*ExponentValue*'.

unitprefixObject = sbiounitprefix('*NameValue*', ...'*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).

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);
```

You can view additional *unitprefixObject* 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 you how to create a user-defined unitprefix, add it to the user-defined library, and query the library.

1 Create a unitprefix.

```
unitprefixObj1 = sbiounitprefix('peta', 15);
```

2 Add the unitprefix to the user-defined library.

```
sbioaddtolibrary(unitprefixObj1);
```

3 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 sbiowhos command.

```
sbiowhos -userdefined -unitprefix

SimBiology UserDefined Unit Prefixes

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

See Also

sbioshowunits, sbiounit, sbioaddtolibrary, sbiowhos

sbiounregisterunit

Purpose

Remove user-defined unit from root and library

Note `sbiounregisterunit` produces a warning and will be removed in a future version. Use `sbioremovefromlibrary` instead.

Syntax

```
sbiounregisterunit('Name')
```

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`, `sbiounitsbiowhos`

Purpose

Remove user-defined unit prefix from root and library

Note `sbiounregisterunitprefix` produces a warning and will be removed in a future version. Use `sbioremovefromlibrary` instead.

Syntax

```
sbiounregisterunitprefix('Name')
```

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

`sbioroot`, `sbioremovefromlibrary`, `sbioshowunitprefixes`, `sbiounitprefix`, `sbiowhos`

sbioupdate

Purpose

Update SimBiology model version

Syntax

```
modelsObj = sbioupdate(modelObj)
simdataObj = sbioupdate(tsObj)
```

Arguments

modelsObj	`sbioupdate` output. Contains array of model objects that includes the top-level model object and a model object for each previously existing submodel.
modelObj	Model object with submodels to be converted into separate model objects.
simdataObj	`sbioupdate` output. Contains SimData object converted from previous time series object.
tsObj	Time series object to be converted to SimData object. Can be a `1-by-n` cell array of timeseries objects

Description

`modelsObj = sbioupdate(`*modelObj*`)` converts a top level SimBiology model object (*modelObj*) that has sub models into an array of SimBiology model objects which do not have any sub models.

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.

Each model created from the previously existing submodel has empty `StatesToLog`, `SpeciesInputFactors`, `ParameterInputFactors` and `SpeciesOutputs` property values.

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*.

Purpose

Construct variant object

Syntax

```
variantObj = ('NameValue')
variantObj = ('NameValue', 'ContentValue')
variantObj = sbiovariant(...'PropertyName', PropertyValue...)
```

Arguments

modelObj	Specify the model object to which you want add a variant.
variantObj	Variant object to create and add to model object.
NameValue	Name of variant object. *NameValue* is assigned to the `Name` property of the variant object.

Description

variantObj = (*'NameValue'*) creates a SimBiology variant object (*variantObj*) with name *NameValue*. The variant object `Parent` property is assigned `[]` (empty).

variantObj = (*'NameValue'*, *'ContentValue'*) creates a SimBiology variant object (*variantObj*) with the `Content` property set to *ContentValue*.

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`.

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).

View properties for a variant object with the `get` command, and modify properties for a variant object with the `set` command. 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)	Append content to variant object
commit (variant)	Commit variant contents to model
copyobj (any object)	Copy SimBiology object and its children
display (any object)	Display summary of SimBiology object
rmcontent (variant)	Remove contents from variant object
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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

Examples

1 Create a variant object

```
variantObj = sbiovariant('p1');
```

2 Add content to the variant that varies a species (`A`) `InitialAmount` property.

```
addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});
```

See Also

`addvariant`, `copyobj`,`getvariant`

sbiowhos

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 the table below:

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 contents of SimBiology project or library defined by `Name`.

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

sbmlexport

Purpose

Export SimBiology model to SBML file

Syntax

```
sbmlexport(modelObj)
sbmlexport(modelObj, 'FileName')
```

Arguments

modelObj	Model object. Enter a variable name for a model object.
FileName	XML file with an Systems Biology Markup Language (SBML) format. Enter either a filename or a path and filename supported by your operating system. If the filename does not have the extension `.xml`, then `.xml` is appended to end of the filename.

Description

`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`.

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 SimBiology” in Getting Started with SimBiology, for more information.

Example

Export a model (`modelObj`) to a file (`gene_regulation.xml`) in the current working directory.

```
sbmlexport(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

sbmlimport, sbiomodel, sbiosaveproject

sbmlimport

Purpose

Import SBML-formatted file

Syntax

```
modelObj = sbmlimport('FileName')
```

Arguments

FileName	XML file with an Systems Biology Markup Language (SBML) format. Enter either a filename or a path and filename supported by your operating system.

Description

`modelObj = sbmlimport('FileName')` imports a 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.

See "SBML Support in SimBiology" in Getting Started with SimBiology, for more information.

Example

```
sbmlobj = sbmlimport('oscillator.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

`sbmlexport`, `sbiosimulate`

MATLAB functions `get` and `set`

3

Methods — By Category

Objects (p. 3-2)	SimBiology objects
Abstract Kinetic Laws (p. 3-2)	Work with abstract kinetic law 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. 3-14)	Command-line syntax for using methods with SimBiology objects

Objects

AbstractKineticLaw object	Kinetic law information in library
Compartment object	Options for compartments
Configset object	Solver settings information for model simulation
Event object	Store event information
KineticLaw object	Kinetic law information for reaction
Model object	Model and component information
Parameter object	Parameter and scope information
Reaction object	Options for model reactions
Root object	Hold models, unit libraries, and abstract kinetic law libraries
Rule object	Hold rule for species and parameters
SimData object	Simulation data storage
Species object	Options for compartment species
Unit object	Holds information about user-defined unit
UnitPrefix object	Holds information about user-defined unit prefix
Variant object	Store alternate component values

Abstract Kinetic Laws

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

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
display (any object)	Display summary of SimBiology object
reorder (model, compartment)	Reorder component lists

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

Events

copyobj (any object)	Copy SimBiology object and its children
display (any object)	Display summary of SimBiology object

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
getparameters (kineticlaw)	Get specific parameters in kinetic law object
getspecies (kineticlaw)	Get specific species in kinetic law object
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
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

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

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
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants

Root

copyobj (any object)	Copy SimBiology object and its children
delete (any object)	Delete SimBiology object
reset (root)	Delete all model objects from root object

Rules

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

SimData

display (any object)	Display summary of SimBiology object
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

Species

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

Units and Unit Prefixes

display (any object)	Display summary of SimBiology object

Variants

addcontent (variant)	Append content to variant object
commit (variant)	Commit variant contents to model
copyobj (any object)	Copy SimBiology object and its children
display (any object)	Display summary of SimBiology object
rmcontent (variant)	Remove contents from variant object
verify (model, variant)	Validate and verify SimBiology model

Using Object Methods

Command-line syntax for using methods with SimBiology objects

Constructing (Creating) Objects (p. 3-14)

Using Object Methods (p. 3-14)

Help for Objects, Methods and Properties (p. 3-15)

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.

```
ObjectName = ConstructorFunction(RequiredParameters,...
                                 'PropertyName',  PropertyValue')
```

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 references by a reaction, us the reaction object methods addkineticlaw, addparameter, addproduct, and addreactant.

```
ObjectName = ReactionName.Method(Arguments)
```

Note, `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.
`sbiohelp('MethodName')`	Display method information.
`sbiohelp('PropertyName')`	Display property information.

4

Methods — Alphabetical List

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

AbstractKineticLaw object

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 relates to the kinetic law object see `KineticLaw 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 MATLAB `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

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

Property Summary

`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
`Tag`	Specify label for SimBiology object
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

See Also

`Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

addcompartment (model, compartment)

Purpose

Create compartment object

Syntax

```
compartmentObj = addcompartment(modelObj, 'NameValue')
compartmentObj = addcompartment(owningCompObj, 'NameValue')
compartmentObj = addcompartment(modelObj, 'NameValue',
   CapacityValue)
compartmentObj = addcompartment(...'PropertyName',
PropertyValue...)
```

Arguments

modelObj	Model object.
owningCompObj	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 object. Enter `double`. Positive real number, default = `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 *PropertyName*. Valid property values are listed on each property reference page.

Description

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 (*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). The property summary on this page shows the list of 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, compartment)	Create compartment object
addspecies (compartment)	Create species object and add to compartment object
copyobj (any object)	Copy SimBiology object and its children
display (any object)	Display summary of SimBiology object
reorder (model, compartment)	Reorder component lists

Property Summary

Properties for compartment objects

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

Examples

1 Create a model object (`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

`addproduct`, `addreactant`, `addreaction`, `addspecies`

MATLAB functions– `get` and `set`

Purpose

Create configuration set object and add to model object

Syntax

```
configsetObj = addconfigset(modelObj, 'NameValue')
configsetObj = addconfigset(..., 'PropertyName',
PropertyValue, ...)
```

Arguments

modelObj	Model object. Enter a variable name.
NameValue	Descriptive name for a configuration set object. Reserved words 'active' and 'default' are not allowed.
configsetObj	Configuration set object.

Description

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 below in the property summary.

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.

You can additionally view configuration set object properties with the command, `get` . You can modify additional configuration set object properties with the command, `set` .

Method Summary

Methods for configuration set objects

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

Property Summary

Properties for configuration set objects

`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
`Type`	Display top-level SimBiology object type

Examples

1 Create a model object by reading the file `oscillator.xml` and add a configuration set that simulates the model for 3000 seconds.

```
modelObj  = sbmlimport('oscillator');
configsetObj = addconfigset(modelObj, 'myset');
```

2 Configure the `configsetObj` `StopTime` to 3000.

```
set(configsetObj, 'StopTime', 3000)
get(configsetObj)
```

```
            Active: 0
    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

Model object methods `getconfigset`, `removeconfigset`, `setactiveconfigset`

MATLAB functions `get` and `set`.

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:

'Type'	'Name'	'PropertyName'
'species'	Name of species. If there are more than one 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 parameter name. If the parameter scope is a kinetic law, specify [reactionName.parameterName].	'Value'
'compartment'	Name of compartment.	'Capacity'

Description

`addcontent(`*variantObj*`, `*contents*`)` adds the data stored in the variable *contents* to the variant object (*variantObj*).

addcontent (variant)

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

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.

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

2 Add a variant object that varies species A `InitialAmount` property.

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});
```

See Also

`addvariant`, `rmcontent`, `sbiovariant`

Purpose

Add event object to model object

Syntax

```
eventObj = addevent(modelObj, 'TriggerValue',
   'EventFcnsValue')
eventObj = addevent(...'PropertyName', PropertyValue...)
```

Arguments

modelObj	Model object.
TriggerValue	Required 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 the table below.
PropertyValue	Property value. For more information on property values see the property reference for each property listed in the Property Summary.

Description

eventObj = addevent(*modelObj*, '*TriggerValue*', '*EventFcnsValue*') creates an event object (*eventObj*) 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 “Events” in the SimBiology User Guide.

`eventObj = addevent(...'PropertyName', PropertyValue...)` defines optional properties. The property name and property value pairs can be any format supported by the function `set` (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
display (any object)	Display summary of SimBiology 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
`Type`	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 = sbmlimport('oscillator')
eventObj = addevent(modelObj, 'time>= 5', 'OpC = 200');
```

2 Get a list of properties for an event object.

```
get(modelObj.Events(1));
```

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'
              Type: 'event'
          UserData: []
```

See Also

`Event object`

addkineticlaw (reaction)

Purpose

Create kinetic law object and add to reaction object

Syntax

```
kineticlawObj = addkineticlaw(reactionObj,
   'KineticLawNameValue')
kineticlawObj= addkineticlaw(..., 'PropertyName',
PropertyValue, ...)
```

Arguments

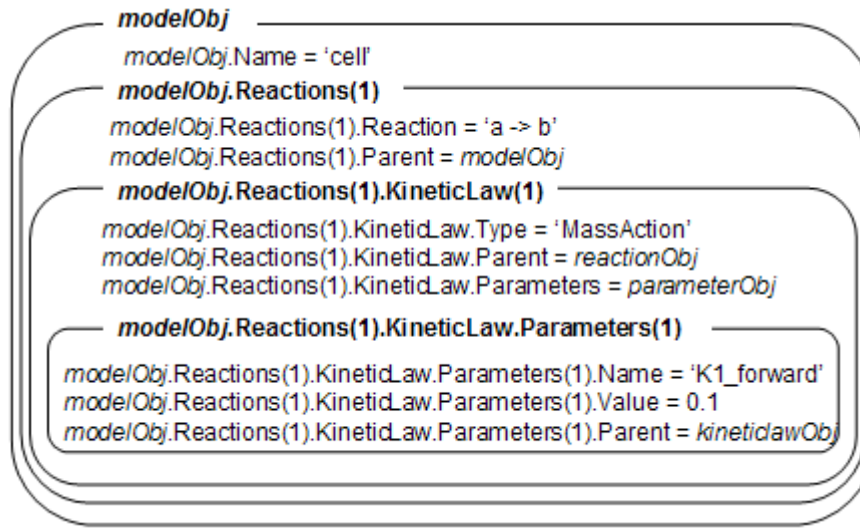
reactionObj	Reaction object. Enter a variable name for a reaction object.
KineticLawNameValue	Property to select the type of kinetic law object to create. For builtin kinetic law valid values are: 'Unknown', 'MassAction', 'Henri-Michaelis-Menten', 'Henri-Michaelis-Menten-Reversible', 'Hill-Kinetics', 'Iso-Uni-Uni', 'Ordered-Bi-Bi', 'Ping-Pong-Bi-Bi', 'Competitive-Inhibition', 'NonCompetitive-Inhibition', 'UnCompetitive-Inhibition'. Find valid *KineticLawNameValue*s 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');
```



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*', *PropertyValue*, ...) constructs a kinetic law object, *kineticlawObj*, and configures *kineticlawObj* 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 kineticlawObj properties are listed below in the property summary.

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(*reactionObj*, 'KineticLaw'). Remove a SimBiology kinetic law object from a SimBiology reaction object with the delete command

Method Summary

Methods for kinetic law objects

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
getparameters (kineticlaw)	Get specific parameters in kinetic law object
getspecies (kineticlaw)	Get specific species in kinetic law object
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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

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)
```

SimBiology 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 paramter 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);
```

SimBiology 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'});
```

SimBiology 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.

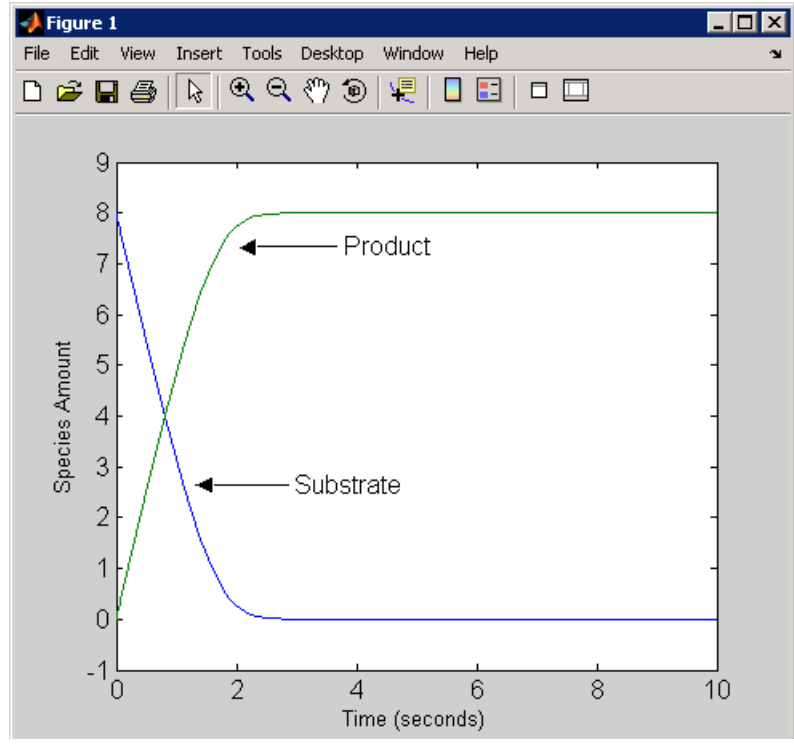
5 Verify that the reaction rate is expressed correctly in the reaction object `ReactionRate` property.

```
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

Example using 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.

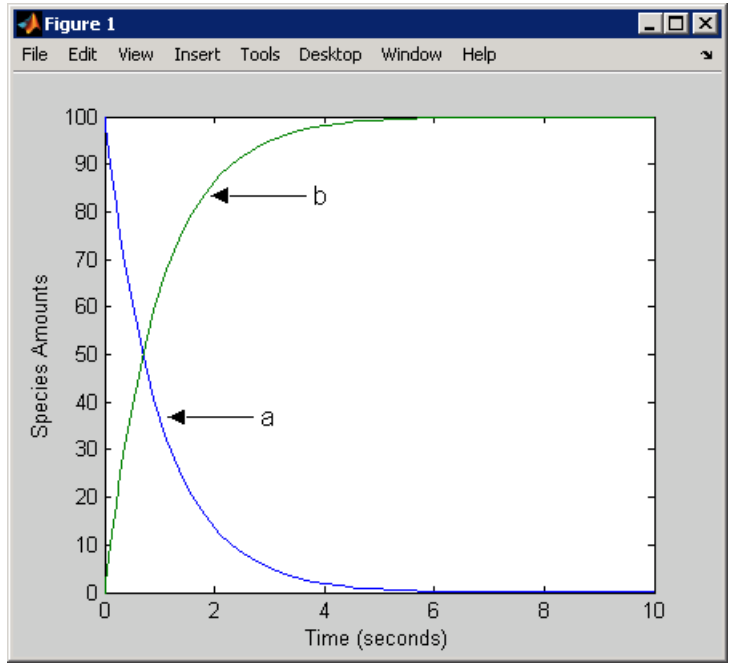
```
parameterObj = addparameter(kineticlawObj, 'k_forward');
set (kineticlawObj, 'ParameterVariablenames', 'k_forward');
get (reactionObj, 'ReactionRate')

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 default value = `1.0`.



See Also

`addreaction`, `setparameter`

Purpose

Add submodel object to model object

Note `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

```
submodelObj = addmodel(modelObj, 'NameValue')
submodelObj = addmodel(...'PropertyName', PropertyValue...)
```

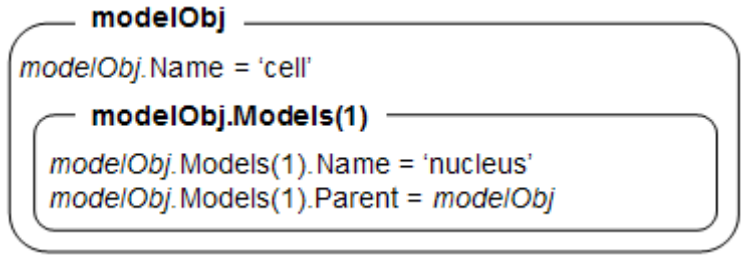
Arguments

modelObj	Model object. Enter a name for a model object.
NameValue	Descriptive name for a model object. Enter a unique character string. A model object can be referenced by other objects using this property.
submodelObj	Model object to be added as submodel.

Description

submodelObj = addmodel(*modelObj*, '*NameValue*') creates a submodel object and returns to *submodelObj*. In the submodel object, this method assigns a value (*NameValue*) to the property `Name`, and assigns the model object (*modelObj*) to the property `Parent`. In the model object, this method assigns the submodel object to the property `Models`.

```
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`

Purpose

Create parameter object and add to model or kinetic law object

Syntax

```
parameterObj = addparameter(Obj, 'NameValue')
parameterObj = addparameter(Obj, 'NameValue', ValueValue)
parameterObj = addparameter(...'PropertyName', PropertyValue...)
```

Arguments

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 see Name.
ValueValue	Property for a parameter object. Enter a number.

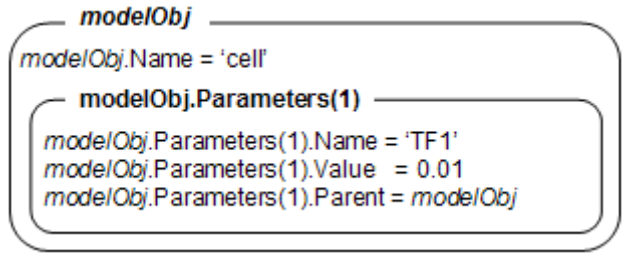
Description

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.

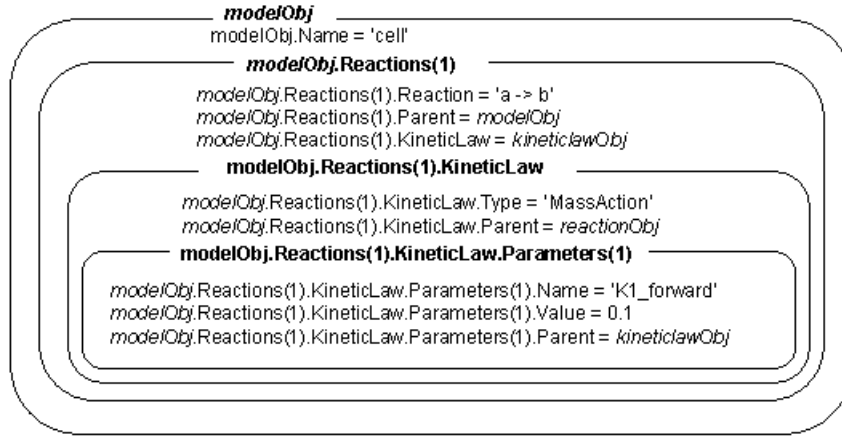
A parameter object defines an assignment that a model, or a kinetic law can use. The scope of the parameter is defined by the parameter parent. If a parameter is defined with a kinetic law object, then only the

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 = 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

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

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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object
`Value`	Assign value to parameter object
`ValueUnits`	Parameter value units

Example

1 Create model object, 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`); 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

% Add parameter with value 0.9 to model object
parameterObj1 = addparameter (modelObj, 'K2', 0.9);

get (modelObj, 'Parameters')
```

MATLAB returns

```
SimBiology Parameter Array

 Index:    Name:    Value:    ValueUnits:
   1         K2       1
```

See Also

`addreaction`

addproduct (reaction)

Purpose

Add product species object to reaction object

Syntax

```
speciesObj = addproduct(reactionObj, 'NameValue')
speciesObj = addproduct(reactionObj, speciesObj)
speciesObj = addproduct(reactionObj, 'NameValue',
   Stoichcoefficient)
speciesObj = addproduct(reactionObj, speciesObj,
   Stoichcoefficient)
```

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`.
speciesObj	Species object.
Stoichcoeffieient	Stoichiometric coefficients for products, length of array equal to length of `NameValue` or length of *speciesObj*.

Description

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,

- 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 create a species object with the function `sbiospecies`, or create and add a species object to a model 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, this method 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, this method 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 SimBiology updates the reaction to use the new name. You must however configure

all other applicable elements such as rules that use the species, and the kinetic law object.

Example

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

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

2 Modify the reaction of the `reactionObj` from `A + C -> U` to `A + C -> U + 2 H`.

```
speciesObj = addproduct(reactionObj, 'H', 2);
```

See Also

`sbiospecies`, `addspecies`

Purpose

Add species object as reactant to reaction object

Syntax

```
speciesObj = addreactant(reactionObj, 'NameValue')
addreactant(reactionObj, speciesObj, Stoichcoeffieient)
addreactant(reactionObj, 'NameValue', Stoichcoeffieient)
```

Arguments

reactionObj	Reaction object.
NameValue	`Name` 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.
speciesObj	Species object or cell array of species objects.
Stoichcoeffieient	Stoichiometric coefficients for reactants, length of array equal to length of `NameValue` or length of *speciesObj*.

Description

speciesObj = addreactant(*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 `Reactants`, 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,

- 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 create a species object with the function `sbiospecies`, or create and add a species object to a model object with the method `addspecies`.

`addreactant(`*`reactionObj`*`, `*`speciesObj`*`, `*`Stoichcoeffieient`*`)`, in the species object (`speciesObj`), this method 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, this method 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 SimBiology updates the reaction to use 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

`sbiospecies`, `addspecies`

addreaction (model)

Purpose

Create reaction object and add to model object

Syntax

```
reactionObj = addreaction(modelObj,'ReactionValue')
reactionObj = addreaction(modelObj, 'ReactantsValue',
   'ProductsValue')
reactionObj = addreaction(modelObj, 'ReactantsValue',
   RStoichCoefficients, 'ProductsValue',
   PStoichCoefficients)
reactionObj = addreaction(...'PropertyName', PropertyValue...)
```

Arguments

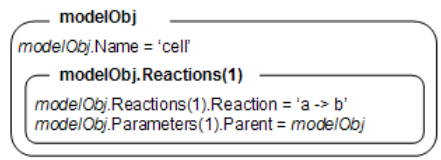
modelObj	SimBiology model object
ReactionValue	Specify the reaction equation. Enter a character string. A hyphen preceded by a space and followed by a right angle bracket (`->`) indicate reactants going forward to products. A hyphen with left and right angle brackets (`<->`) indicate a reversible reaction.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

Description

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 Reactions, and returns the reaction object (reactionObj).

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



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 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`.

`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).

Method Summary

Methods for reaction objects

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
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants

Property Summary

Properties for reaction objects

`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
`Type`	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, 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

```
ruleObj = addrule(modelObj, 'RuleValue')
ruleObj = addrule(modelObj, 'RuleValue', 'RuleTypeValue')
ruleObj = addrule(..., 'PropertyName', PropertyValue,...)
```

Arguments

modelObj	Model object to which to add the rule.
RuleValue	Enter a character string within quotes. 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).

View additional rule properties with the function `get`, and modify rule properties with the function `set`. Copy a rule object to a model with the function `copyobj`, or delete a rule object from a model with the function `delete`.

Method Summary

Methods for rule objects

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

Property Summary

Properties for rule objects

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

Examples

Add a rule with default `RuleType`.

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

```
modelObj = sbiomodel('cell');
ruleObj = addrule(modelObj, 'O.1*B-A')
```

2 Get a list of properties for a rule object.

```
get(modelObj.Rules(1)) or get(ruleObj)
```

MATLAB displays a list of rule properties.

```
    Active: 1
    Annotation: ''
          Name: ''
         Notes: ''
        Parent: [1x1 SimBiology.Model]
          Rule: 'O.1*B-A'
      RuleType: 'algebraic'
           Tag: ''
          Type: 'rule'
      UserData: []
```

Add rule with `RuleType` property set to `rate`.

1 Create model object, 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 -> 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: ''
     Notes: ''
    Parent: [1x1 SimBiology.Model]
      Rule: 'c = k*(a+b)'
  RuleType: 'rate'
       Tag: ''
      Type: 'rule'
  UserData: []
```

See Also

`copyobj`, `delete`, `sbiomodel`

addspecies (compartment)

Purpose

Create species object and add to compartment object

Syntax

```
speciesObj = addspecies(compObj, 'NameValue')
speciesObj = addspecies(compObj, 'NameValue',
   InitialAmountValue)
speciesObj = addspecies(...'PropertyName', PropertyValue...)
```

Arguments

compObj	Compartment object.
NameValue	Name for a species object. Enter a character string unique within *compObj*. 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.
IntialAmountValue	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 *PropertyName*. Valid property values are listed on each property reference page.

Description

speciesObj = addspecies(*compObj*, '*NameValue*') creates 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, this method 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 H2O. However, another compartment can have a species named H2O.

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 **Output** pane opens with the results of **Find**. Double-click a result row to go to the location of the model component.

SimBiology automatically updates species names for reactions that use `MassAction` kinetic law.

Method Summary

Methods for species objects

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

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
`Tag`	Specify label for SimBiology object

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

Examples

Add two species to a model, one is a reactant and the other is the enzyme catalyzing the reaction.

1 Create a model object with the name `my_model` and add a compartment object.

```
modelObj = sbiomodel ('my_model');
compObj = addcompartment(modelObj, 'comp1');
```

2 Add two species objects with the names `glucose_6_phosphate` and `glucose_6_phosphate_dehydrogenase`.

```
speciesObj1 = addspecies (compObj, 'glucose_6_phosphate');
speciesObj2 = addspecies (compObj, ...
                          'glucose_6_phosphate_dehydrogenase');
```

3 Set initial amount of `glucose_6_phosphate` to `100` and verify.

```
set (speciesObj1, 'InitialAmount',100);
get (speciesObj1, 'InitialAmount')
```

MATLAB returns

```
ans =

   100
```

4 Use `get` to note that `modelObj` contains the species object array.

```
get(compObj, 'Species')
```

MATLAB returns,

```
SimBiology Species Array

   Index:    Name:                                 InitialAmount:
   1         glucose_6_phosphate                   100
   2         glucose_6_phosphate_dehydrogenase     0
```

5 Retrieve information about the first species in the array.

```
get(compObj.Species(1))
            Annotation: ''
     BoundaryCondition: 0
        ConstantAmount: 0
         InitialAmount: 100
    InitialAmountUnits: ''
                  Name: 'glucose_6_phosphate'
                 Notes: ''
                Parent: [1x1 SimBiology.Compartment]
                   Tag: ''
                  Type: 'species'
              UserData: []
```

See Also

`addcompartment`, `addproduct`, `addreactant`, `addreaction`

MATLAB functions– `get` and `set`

Purpose

Add variant to model

Syntax

```
variantObj = addvariant(modelObj, 'NameValue')
variantObj2 = addvariant(modelObj, variantObj)
```

Arguments

modelObj	Specify the model object to which you want add a variant.
variantObj	Variant object to create and add to model object.
NameValue	Name of variant object. *NameValue* is assigned to the Name property of the variant object.

Description

variantObj = addvariant(*modelObj*, '*NameValue*') creates a SimBiology variant object (*variantObj*) with name *NameValue* and adds the variant object to the SimBiology model object *modelObj*. The variant object Parent property is assigned the value of *modelObj*.

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants see Variant object.

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*.

View properties for a variant object with the get command, and modify properties for a variant object with the set command. 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.

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

2 Add a variant object that varies species A `InitialAmount` property

```
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 MATLAB `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

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
`Type`	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, modelObj)`

Arguments

modelObj	Specify the model object to which you want to commit a variant.
variantObj	Variant object to commit to model object.

Description

`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 replaces the values stored in the model.

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants see `Variant object`.

The `Contents` are set on the model object in order of occurrence, with duplicate entries overwriting. If the `commit` method finds an incorrectly specified entry, an error occurs and the remaining properties defined in the `Contents` property are not set.

Examples

1 Create a model containing one species.

```
modelObj = sbiomodel('mymodel');
compObj = addcompartment(modelObj, 'comp1');
speciesObj = addspecies(compObj, 'A', 10);
```

2 Add a variant object that varies species A `InitialAmount` property

```
variantObj = addvariant(modelObj, 'v1');
addcontent(variantObj, {'species', 'A', 'InitialAmount', 5});
```

3 Commit the contents of the variant (*variantObj*).

```
commit (variantObj, modelObj);
```

See Also

Variant object, addvariant

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` using 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 way compartments are organized in your model without invalidating any expressions.

To add species that participate in reactions, add the reaction to the model using the `addreaction` method. When you define a reaction with a new species,

- if no compartment objects exist in the model, the `addreaction` method creates a compartment object (called `'unnamed'`) in the model and adds the newly created species to that compartment.
- if only one compartment object exists in the model, the method creates a species object in that compartment.
- if there is more than one compartment object 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`.

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 MATLAB `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

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
display (any object)	Display summary of SimBiology object
reorder (model, compartment)	Reorder component lists

Property Summary

Properties for compartment objects

`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
`Type`	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

Obj

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

parentObj

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, abstract kinetic law object	`sbioroot`

modelObj

Model object to be copied.

copiedObj

Output returned by `copyobj` method with 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`.

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.

Example

Create a reaction object separate from a model object and then add it to a model.

1 Create a model object and create a separate reaction object.

```
modelObj = sbiomodel('cell');
reactionObj = sbioreaction('a -> b');
```

2 Create a copy of the reaction object and assign it to the model object.

```
reactionObjCopy = copyobj(reactionObj, modelObj);
modelObj.Reactions

SimBiology Reaction Array

Index:    Reaction:
 1         a -> b
```

See Also

sbiomodel, sbioreaction, sbioroot

delete (any object)

Purpose

Delete SimBiology object

Syntax

```
delete(Obj)
```

Arguments

Obj	SimBiology object: abstract kinetic law, configuration set, kinetic law, model, parameter, reaction, rule, or species.

Description

`delete(Obj)` removes an object (*Obj*) from its parent.

- 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 before you can delete the species object.
- If *Obj* 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.
- If *Obj* 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 *Obj* is an abstract kinetic law object and there is a kinetic law object referencing it, this method returns an error.
- If *Obj* 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, 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 *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

```
modelObj = sbiomodel('cell')
reactionObj = addreaction(modelObj, 'A + B -> C')
```

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 "Events" in the SimBiology User Guide.

See "Property Summary" on page 4-71 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 MATLAB `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
sbioevent	Construct event object

Method Summary

copyobj (any object)	Copy SimBiology object and its children
display (any object)	Display summary of SimBiology 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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

See Also

`AbstractKineticLaw object`, `Configset object`, `KineticLaw object`, `Model objectParameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Purpose

Get adjacency matrix from model object

Syntax

```
M = getadjacencymatrix(modelObj)
M = getadjacencymatrix(modelObj,'flat')
[M,Headings] = getadjacencymatrix(modelObj)
[M, Headings, Mask]=getadjacencymatrix(modelObj)
```

Arguments

M	Adjacency matrix for *modelObj*
modelObj	Specify model object.
`'flat'`	Return adjacency matrix for only specified *modelObj* not for objects contained in the *modelObj*
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`.
Mask	Returns `1` for species object `0` for reaction object to *Mask*

Description

`getadjacencymatrix` returns adjacency matrix for model object.

M = `getadjacencymatrix(`*modelObj*`)` returns adjacency matrix for model object, (*modelOBJ*) to *M*.

An adjacency matrix is defined by listing all species contained by *modelObj* and all reactions contained by *modelObj* 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.

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*.

[*M*,*Headings*] = getadjacencymatrix(model*Obj*) returns the adjacency matrix to M and the row and column headings to *Headings*. *Headings* is defined by listing all Name property values of species contained by *modelObj* and all Name property values of reactions contained by *modelObj*.

[*M*, *Headings*, *Mask*]=getadjacencymatrix(*modelObj*) returns an array of ones and zeros to *Mask* where a 1 represents a species object and a 0 represents a reaction object.

Examples

1 Read in a model using sbmlimport.

```
modelObj = sbmlimport('lotka.xml');
```

2 Get the adjacency matrix for the modelObj.

```
[M, Headings] = getadjacencymatrix(modelObj)
```

See Also

getstoichmatrix

Purpose

Get configuration set object from model object

Syntax

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

Arguments

modelObj	Model object. Enter a variable name for a model object.
NameValue	Name of the `configset` object.
configsetObj	Object holding the simulation specific information.

Description

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*.

configsetObj = `getconfigset(`*modelObj*`,'active')` retrieves the active configuration set.

A configuration set object stores simulation specific information. A SimBiology model can contain multiple `configsets` with one being active at any given time. The active configuration set contains the settings that are used during the simulation.

Use the `setactiveconfigset` function to define the active configset. *modelObj* always contains at least one configset object with name configured to 'default'. Additional configset objects can be added to *modelObj* with the method, `addconfigset` .

Example

1 Retrieve the default`configset` object from the `modelObj`.

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

See Also

`addconfigset`, `removeconfigset`, `setactiveconfigset`

Purpose

Get data from SimData object array

Syntax

```
[t, x, names] = getdata(simDataObj)
[Out] = getdata(simDataObj, 'FormatValue')
```

Arguments

Output Arguments

t	An n-by-1 vector of time points.
x	An n-by-m data array. *t* and *names* label the rows and columns of *x* respectively.
names	An m-by-1 cell array of names.
Metadata	When used with the 'nummetadata' input argument, *Metadata* contains a cell array of metadata structures. The elements of *Metadata* label the columns of *x*.
Out	Data returned in format as specified in '*FormatValue*', shown in "Input Arguments" on page 4-78. Depending on specified '*FormatValue*', *Out* contains one of the following: • Structure array • SimData object • Time series object • Combined time series object from array of SimData objects.

Input Arguments

simDataObj	SimData object. Enter a variable name for a SimData object.
FormatValue	Chose a format from the table below.

Available values for *FormatValue*:

FormatValue	Description
'num'	Specifies the format that lets you return data in numeric arrays. This is the default when getdata is called with two or more 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 *names* 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.

FormatValue	Description
'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.
'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 4-78.

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 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

SimBiology methods: `displayresample`, `selectselectbyname`, `setactiveconfigset`

MATLAB functions `get`, `struct`,

Purpose

Get specific parameters in kinetic law object

Syntax

```
parameterObj = getparameters(kineticlawObj)
parameterObj = getparameters(kineticlawObj,
   'ParameterVariablesValue")
```

Arguments

kineticlawObj	Retrieve parameters used by kinetic law object.
ParameterVariablesValue	Retrieve parameters used by kinetic law object corresponding to the specified parameter in `ParameterVariables` property of the kinetic law object.

Description

parameterObj = `getparameters(`*kineticlawObj*`)` returns the parameters used by the kinetic law object `kineticlawObj` to `parameterObj`.

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.

If you change the name of a parameter you must configure all applicable elements such as rules that use the parameter, any user specified `ReactionRate`, or the kinetic law object property `ParameterVariableNames`. Use the method `setparameter` to configure `ParameterVariableNames`.

Example

Create a model, add a reaction and assign the `ParameterVariableNames` 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 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)
[T,R, Outputs, InputFactors] = getsensmatrix(simDataObj,
   OutputNames,InputFactorNames)
```

Arguments

T	*T* is `m by 1` array specifying time points for the sensitivity data in R.
R	*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}`.
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 input factors. Where input factors are the names of the states with respect to which you want to calculate sensitivity.

Description

`[`*T,R, Outputs, InputFactors*`] = getsensmatrix(`*simDataObj*`)` gets time and sensitivity data from the SimData object (*simDataObj*).

When *simDataObj* contains more than one element, the output arguments are cell arrays in which each cell contains data for the corresponding element of *simDataObj*.

The `getsensmatrix` method can only return sensitivity data that is contained in the `SimData` object. The sensitivity data that is logged in a `SimData` object is set at simulation time by the configuration set used during the simulation. This is typically the model's active configuration set. See Sensitivity Analysis in the SimBiology User's Guide for an explanation of how to set up a sensitivity calculation using 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);
      ```

   c. 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

SimBiology methods: `display`, `getdata`, `resample`, `selectbyname`

MATLAB functions get, struct

Purpose

Get specific species in kinetic law object

Syntax

```
speciesObj = getspecies(kineticlawObj)
speciesObj = getspecies(kineticlawObj,
   'SpeciesVariablesValue')
```

Arguments

kineticlawObj	Retrieve species used by kinetic law object.
SpeciesVariablesValue	Retrieve species used by kinetic law object corresponding to the specified species in the `SpeciesVariables` property of the kinetic law object.

Description

speciesObj = `getspecies(`*kineticlawObj*`)` returns the species used by the kinetic law object `kineticlawObj` to `speciesObj`.

speciesObj = `getspecies(`*kineticlawObj*`, '`*SpeciesVariablesValue*`')` returns the species in the `SpeciesVariableNames` property to `speciesObj`.

`SpeciesVariablesValue` is the name of the species as it appears in the `SpeciesVariables` property of `kineticlawObj`. `SpeciesVariablesValue` can be a cell array of strings.

Species names are referenced by reaction objects, kinetic law objects, and model objects. If you change the name of a species SimBiology updates the reaction to use the new name. You must however configure all other applicable elements such as rules that use the species, and the kinetic law object `SpeciesVariableNames`. Use the method `setspecies` to configure `SpeciesVariableNames`.

Example

Create a model, then add a reaction, and assign the `SpeciesVariableNames` for the reaction rate equation.

1 Create model object, 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 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     a        0
```

See Also

`addspecies`, `setspecies`, `getparameters`, `setparameter`

Purpose

Get stoichiometry matrix from model object

Syntax

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

Arguments

M	Adjacency matrix for *modelObj*.
modelObj	Specify model object *modelObj*.
'flat'	Return stoichiometry matrix for only specified *modelObj* not for objects contained in the *Obj*.
objSpecies	Return list of *modelObj* species by Name property of 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 list of *modelObj* reactions by Name property of reactions.

Description

getstoichmatrix returns a stoichiometry matrix for a model object.

M = getstoichmatrix(*modelObj*)returns a stoichiometry matrix for SimBiology a model object, (*modelObj*) to *M*.

A stoichiometry matrix is defined by listing all reactions contained by *modelObj* column-wise and all species contained by *modelObj* 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:

```
        A     B     C    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'}.

Example

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	Variant object returned by `getvariant` method.
modelObj	Model object from which to get variant.
'*NameValue*'	Name of the variant to get from the model object *modelObj*.

Description

variantObj = `getvariant(`*modelObj*`)` returns SimBiology variant objects contained by 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 name, *NameValue*, contained by 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. 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 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 several variants.

```
modelObj = sbiomodel('mymodel');
variantObj1 = addvariant(modelObj, 'v1');
variantObj2 = addvariant(modelObj, 'v2');
```

2 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.

```
vObjv2 = getvariant(modelObj, 'v2');
```

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, SimBiology 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. SimBiology 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. SimBiology 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.

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

   SimBiology 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 4-98

Properties define the characteristics of an object. Use the MATLAB `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 4-94.

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:

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

In SimBiology `Henri-Michaelis-Menten` is a built-in abstract kinetic law, where V_m and K_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 Getting Started with SimBiology 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'});
```

SimBiology now assigns the rate equation in the reaction object as follows:

Va*A/(Ka + A)

For a detailed procedure, see “Examples” on page 4-99.

The following table below 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: $V_m * S/(K_m + S)$	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.
`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.

Property	Property Purpose	Abstract Kinetic Law Object	Kinetic Law Object
`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

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
getparameters (kineticlaw)	Get specific parameters in kinetic law object
getspecies (kineticlaw)	Get specific species in kinetic law object
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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

Examples

This example shows how to define the reaction rate for a reaction in SimBiology.

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

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

2 Define a kinetic law for the reaction object.

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

3 Query the parameters and species variables defined in the kinetic law.

```
get(kineticlawObj, 'ParameterVariables')

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 names Va, Ka, and 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 component 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 4-102 for links to model property reference pages.

Properties define the characteristics of an object. Use the MATLAB `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

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

Property Summary

`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
`Tag`	Specify label for SimBiology object
`Type`	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`

Parameter object

Purpose

Parameter and scope information

Description

The parameter object represents a *parameter*, which is a quantity that can change or can be constant. In 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 4-105 for links to parameter object property reference pages.

Properties define the characteristics of an object. Use the MATLAB `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
sbioparameter	Construct parameter 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

Property Summary

`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
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object
`Value`	Assign value to parameter object
`ValueUnits`	Parameter value units

See Also

`AbstractKineticLaw object`, `Configset objectKineticLaw object`, `Model object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Reaction object

Purpose

Options for model reactions

Description

The reaction object represents a *reaction*, 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 H2O
```

Spaces are required before and after species names and stoichiometric values.

See “Property Summary” on page 4-107 for links to reaction object property reference pages.

Properties define the characteristics of an object. Use the MATLAB `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
sbioreaction	Construct reaction 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
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants

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
`Tag`	Specify label for SimBiology object

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

See Also

`AbstractKineticLaw object`, `Configset objectKineticLaw object`, `Model object`, `Parameter object`, `Root object`, `Rule object`, `Species object`

Purpose

Remove configuration set from model

Syntax

```
removeconfigset(modelObj, 'NameValue')
removeconfigset(modelObj, configsetObj)
```

Arguments

modelObj	Model object from which to remove configuration set.
NameValue	Name of the configuration set.
configsetObj	Configuration set object that is to be removed from model object

Description

`removeconfigset(modelObj, 'NameValue')` removes the configset object with name, *NameValue* from 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.

`removeconfigset(modelObj, configsetObj)` removes the configuration set object, *configsetObj* from SimBiology model, *modelObj*. The configuration set is not deleted; if you want to delete `configsetObj` use the `delete` method.

If however, there is no MATLAB variable holding the configset, `removeconfigset(modelObj, 'NameValue')`, removes the configset from the model and deletes it.

Example

1 Create a model object by importing the file `oscillator.xml` and add a configset.

```
modelObj  = sbmlimport('oscillator');
```

```
configsetObj = addconfigset(modelObj, 'myset');
```

2 Remove the configset from `modelObj` by name or alternatively by indexing.

```
% Remove the configset with name 'myset'.
  removeconfigset(modelObj, 'myset');

 % Get all configset objects and remove the second.
  configsetObj = getconfigset(modelObj);
  removeconfigset(modelObj, configsetObj(2));
```

See Also

`addconfigset`, `getconfigset`, `setactiveconfigset`

Purpose

Remove variant from model

Syntax

```
variantObj = removevariant(modelObj, 'NameValue')
variantObj = removevariant(modelObj, variantObj)
```

Arguments

modelObj	Specify the model object from which you want to remove variant.
variantObj	Specify the variant object to return from the model object.

Description

variantObj = removevariant(*modelObj*, '*NameValue*') removes a SimBiology variant object with 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.

variantObj = removevariant(*modelObj*, *variantObj*) removes a SimBiology variant object (*variantObj*) returns the variant object *variantObj*.

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

Examples

1 Create a model containing several variants.

```
modelObj = sbiomodel('mymodel');
variantObj1 = addvariant(modelObj, 'v1');
variantObj2 = addvariant(modelObj, 'v2');
variantObj3 = addvariant(modelObj, 'v3');
```

2 Remove a variant object using its name.

```
removevariant(modelObj, 'v1');
```

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
```

b Remove the variant object

```
removevariant(modelObj, vObjs(2));
```

See Also

`addvariant`, `getvariant`

Purpose

Reorder component lists

Syntax

```
modelObj = reorder(Obj, NewOrder)
```

Arguments

Obj	Model object or compartment. Enter a variable name.
NewOrder	Object vector in the new order. If *Obj* is a model object, *NewOrder* can be an array of compartments, events, parameters, reactions or rules objects. If *Obj* is an compartment object, *NewOrder* must be an array of species objects.

Description

modelObj = reorder(*Obj*, *NewOrder*) reorders the component vector *NewOrder*, to be in the order specified.

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

1 Import a model

```
modelObj = sbmlimport('lotka');
```

2 Display the order of the reactions in the model.

```
get(modelObj.Reactions);
```

```
   SimBiology Reaction Array

   Index:    Reaction:
   1         x + y1 -> 2 y1 + x
   2         y1 + y2 -> 2 y2
   3         y2 -> z
```

3 Reverse the order of the reaction in the model.

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

Purpose

Resample SimData object array onto new time vector.

Syntax

```
newSimDataObj = resample(simDataObj)
newSimDataObj = resample(simDataObj, timevector)
newSimDataObj = resample(simDataObj, timevector, method)
```

Arguments

newSimDataObj	Resampled SimData object array
simDataObj	SimData object array that you want to resample
timevector	Real numeric array of time points onto to which you want to resample the data.

method	Method to use during resampling. Can be one of the following:
	• `'interp1q'` – uses the MATLAB function `interp1q`.
	• – To use the MATLAB function `interp1`, specify one of the following methods:
	  - `'nearest'`
	  - `'linear'`
	  - `'spline'`
	  - `'pchip'`
	  - `'cubic'`
	  - `'v5cubic'`
	• `'zoh'` – specifies zero-order hold.

Description

newSimDataObj = `resample(`*simDataObj*`)` resamples the simulation data contained in every element of the SimData object array *simDataObj* onto a common time vector, producing a new SimData array *newSimDataObj*. By default, the common time vector is taken from the element of *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, SimBiology 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 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 ensemble run.

```
csObj  = getconfigset(m1);
```

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

3 Interpolate time steps.

```
newSimDataObj = resample(simDataObj, [1:10], 'linear');
```

4 View 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

1 Query `sbioroot` that 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
```

2 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, sbioregisterunit, sbioregisterunitprefix, sbioroot, sbioreset, sbiohelp

rmcontent (variant)

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* are shown below:

'Type'	'Name'	'PropertyName'
`'species'`	Name of species. If there are more than one 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 parameter name. If the parameter scope is a kinetic law, specify [`reactionName.parameterName`].	`'Value'`
`'compartment'`	Name of 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**.

rmcontent (variant)

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:
   1                 species      A                 InitialAmount
   2                 species      B                 InitialAmount
   3                 species      C                 InitialAmount
```

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:
    1                 species      A                 InitialAmount
    2                 species      C                 InitialAmount
```

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:
   1                 species      C                 InitialAmount
```

See Also

addvariant, rmcontent, sbiovariant

rmproduct (reaction)

Purpose

Remove species object from reaction object products

Syntax

```
rmproduct(reactionObj, SpeciesName)
rmproduct(reactionObj, speciesObj)
```

Arguments

reactionObj	Reaction object.
SpeciesName	Name for a model object. Enter a species name or cell array of species names.
speciesObj	Species object. Enter a species object or an array of species objects.

Description

`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.

`rmproduct(reactionObj, speciesObj)` removes a species object as described above using 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 will be returned.

Examples

Example 1

Shows you how to remove a product that was previously added to a reaction. You can remove the species object using the species name.

```
modelObj = sbiomodel('cell');
reactionObj = addreaction(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

rmreactant (reaction)

Purpose

Remove species object from reaction object reactants

Syntax

```
rmreactant(reactionObj, SpeciesName)
rmreactant(reactionObj, speciesObj)
```

Arguments

reactionObj	Reaction object.
SpeciesName	Name for a species object. Enter a species name or cell array of species names.
speciesObj	Species object. Enter a species object or an array of species objects.

Description

`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 model index 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 method, `delete` to remove it from the parent object.

If one of the species specified does not exist as a reactant, a warning is returned.

Examples

Example 1

Shows you 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 -> creatine + ATP');
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

`rmproduct`, `delete`

Root object

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 builtin (`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 4-128 for links to root object property reference pages.

Properties define the characteristics of an object. Use the MATLAB `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
delete (any object)	Delete SimBiology object
reset (root)	Delete all model objects from root object

Property Summary

`BuiltInLibrary`	Library of built-in components
`Models`	Contain all model objects

`Type`	Display top-level SimBiology object type
`UserDefinedLibrary`	Library of user-defined components

See Also

`AbstractKineticLaw object`, `Configset objectKineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Rule object`, `Species object`

Rule object

Purpose

Hold rule for species and parameters

Description

The SimBiology rule object represents a *rule*, which is a mathematical expression that modifies a species amount or a parameter value. To see a description of the types of SimBiology rules, see `RuleType`

See “Property Summary” on page 4-130 for links to rule property reference pages.

Properties define the characteristics of an object. Use the MATLAB `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
sbiorule	Construct rule 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

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

See Also

`AbstractKineticLaw object`, `Configset objectKineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Species object`

select (SimData)

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 `names` label the rows and columns of `x` respectively.
`names`	An `m-by-1` cell array of names.

`Out`	Data returned in format as specified in `'FormatValue'`, shown in "Input Arguments" on page 4-133. Depending on specified `'FormatValue'`, `Out` contains one of the following: • Structure array • SimData object • Time series object • Combined time series object from array of SimData objects.

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 Chose a format from the table below.

Available values for *FormatValue*:

FormatValue	Description
`'num'`	Specifies the format that lets you return data in numeric arrays. This is the default when `select` is called with two or more 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*.

FormatValue	Description
`'numqualnames'`	Specifies the format that lets you return qualified names in *`names`* 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

`[t,x,names] = select(simDataObj, Query)` returns simulation time and state data from the SimData object (`simDataObj`) that matches the query argument *`Query`*.

In a SimData object *`simDataObj`*, 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 *`simDataObj`*, use the syntax `[t, x, names] = select (simDataObj, {'Type', 'parameter'}]`.

`[Out] = select(simDataObj, Query, 'Format', 'FormatValue'))` returns the data in the specified format. Valid formats are listed in "Input Arguments" on page 4-133.

Examples

These examples show you 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
```

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

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

3 Select all species data logged in the SimData array sdarray.

```
[t x n] = select(simDataObj, {'Type','species'});
```

4 Select data for the parameters with name 'Kd' and return the results in a new SimData object array.

```
newsd = select(simDataObj, {'Type','parameter','name', 'Kd'});
```

5 This selects all data from `simDataObj` with a name that matches the pattern 'G' and returns time series objects.

```
ts = select(simDataObj, {'Where','Name','regexp','G'}, ...
                        'Format','ts');
```

See Also

`sbioselect`, `sbiosimulate`, `Simdata object`, `getdata`, `selectbyname`.

Purpose

Set active configuration set for model object

Syntax

```
configsetObj = setactiveconfigset(modelObj, 'NameValue')
configsetObj2 = setactiveconfigset(modelObj, configsetObj1)
```

Description

`configsetObj = setactiveconfigset(modelObj, 'NameValue')` sets the configuration set *NameValue* to be the active configuration set for the model *modelObj* and returns to *configsetObj*.

`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.

The active configuration set contains the settings that are be used during a simulation. A default configuration set is attached to any new model.

Examples

1 Create a model object by importing the file `oscillator.xml` and add a configset that simulates for 3000 seconds.

```
modelObj  = sbmlimport('oscillator');
configsetObj = addconfigset(modelObj, 'myset');
```

2 Configure the `configsetObj` `StopTime` to `3000`.

```
set(configsetObj, 'StopTime', 3000)
get(configsetObj)
```

```
            Active: 0
    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`

Purpose

Select data by name from SimData object array

Syntax

```
[t,x,n] = selectbyname(simDataObj, 'NameValue')
Out = selectbyname(simDataObj, NameValue, 'Format', Format)
```

Arguments

Output Arguments

t	An n-by-1 vector of time points.
x	An n-by-m data array. *t* and *names* label the rows and columns of *x* respectively.
n	An m-by-1 cell array of names.

Out	Data returned in format as specified in '*FormatValue*', shown in "Input Arguments" on page 4-133. Depending on specified '*FormatValue*', *Out* contains one of the following: • Structure array • SimData object • Time series object • Combined time series object from array of SimData objects.

Input Arguments

simDataObj	SimData object array. Enter a variable name for a SimData object.
NameValue	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	Chose a format from the table below.

Available values for *FormatValue*:

FormatValue	Description
`'num'`	Specifies the format that lets you return data in numeric arrays. This is the default when `select` is called with two or more 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 *`names`* 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 labelling 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 4-140.

Example

```
% 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 arra
s = selectbyname(sdarray,{'RexGFP';'nuc.GFP';'cytosol.GFP'},...
                         'Format','struct');
```

See Also

`getdata`, `sbioselect`, `sbiosimulate`

setparameter (kineticlaw)

Purpose

Specify specific parameters in kinetic law object

Syntax

```
setparameter(kineticlawObj, 'ParameterVariablesValue',
   'ParameterVariableNamesValue')
```

Arguments

ParameterVariableValue	Specify value of parameter variable in kinetic law object.
ParameterVariableNamesValue	Specify the parameter name with which to configure parameter variable in kinetic law object. Determines parameters in `ReactionRate` equation.

Description

Configure `ParameterVariableNames` in 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`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`.

Example

Create a model, add a reaction, and assign the `ParameterVariableNames` 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 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 species variable in kinetic law object.
SpeciesVariableNamesValue	Specify the species name with which to configure species variable in kinetic law object. Determines species in `ReactionRate` equation

Description

`setspecies` configures kinetic law object `SpeciesVariableNames` property.

`setspecies(kineticlawObj, 'SpeciesVariablesValue', 'SpeciesVariableNamesValue')` configures the `SpeciesVariableNames` property of the kinetic law object, `kineticlawObj`. `SpeciesVariablesValue` corresponds to one of the strings in `SpeciesVariables` property of `kineticlawObj`. The corresponding 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`.

Example

Create a model, add a reaction and assign the `SpeciesVariableNames` 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 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 shown in the "Property Summary" on page 4-149 below. Properties define the characteristics of an object. Use the MATLAB `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 the "Method Summary" on page 4-148 below.

Constructor Summary

`sbioensemblerun`	Multiple stochastic ensemble runs of SimBiology model
`sbiosimulate`	Simulate model object

Method Summary

display (any object)	Display summary of SimBiology object
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
`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`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`, `Species object`

Species object

Purpose

Options for compartment species

Description

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.

To add species that participate in reactions, add the reaction to the model. SimBiology creates a compartment object (*`unnamed`*) and the necessary species objects.

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.

See “Property Summary” on page 4-151 for links to species property reference pages. Properties define the characteristics of an object. Use the MATLAB `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

addspecies (compartment)	Create species object and add to compartment object
sbiospecies	Construct species object

Method Summary

Methods for species objects

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

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
`Tag`	Specify label for SimBiology object
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

See Also

`Compartment object`, `Configset object`, `KineticLaw object`, `Model object`, `Parameter object`, `Reaction object`, `Root object`, `Rule object`

Unit object

Purpose

Holds 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 `Composition`, to specify the composition of your units. See "Property Summary" on page 4-152 for links to unit object property reference pages.

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

Constructor Summary

`sbiounit`	Create user-defined unit

Method Summary

display (any object)	Display summary of SimBiology object

Property Summary

`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

`Tag`	Specify label for SimBiology object
`Type`	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

Holds 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 exponent of your unit prefix. See "Property Summary" on page 4-154 for links to unit prefix object property reference pages.

Properties define the characteristics of an object. Use the MATLAB `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 **Unit Manager** in the SimBiology desktop.

Constructor Summary

`sbiounitprefix`	Create user-defined unit prefix

Method Summary

display (any object)	Display summary of SimBiology object

Property Summary

`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
`Tag`	Specify label for SimBiology object

`Type`	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`, `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 4-157 for links to species property reference pages. Properties define the characteristics of an object. Use the MATLAB `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

addcontent (variant)	Append content to variant object
commit (variant)	Commit variant contents to model
copyobj (any object)	Copy SimBiology object and its children
display (any object)	Display summary of SimBiology object
rmcontent (variant)	Remove contents from variant object
verify (model, variant)	Validate and verify SimBiology model

Property Summary

Properties for variant objects

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

See Also

Objects — `Compartment objectConfigset object`, `Model object`, `Parameter object`, `Species object`

Functions — `sbiosimulate`

Purpose

Validate and verify SimBiology model

Syntax

```
verify(modelObj)
verify(modelObj, configsetObj)
verify(modelObj, variantObj)
verify(modelObj, configsetObj, variantObj)
```

Description

`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.

`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.

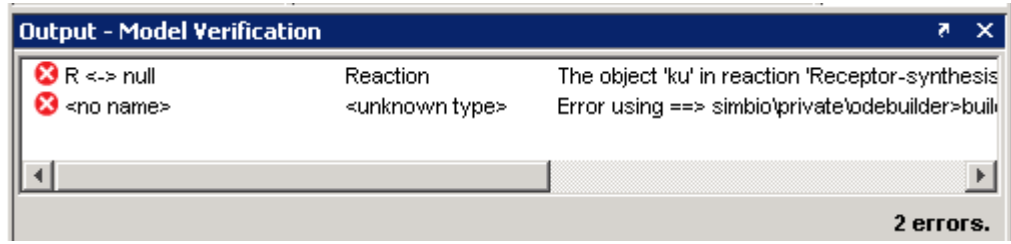
`verify(modelObj, variantObj)` performs checks on the variant object (*`variantObj`*) in conjunction with the model object (*`modelObj`*) to verify that you can simulate the model. The model object is required for the verification of the variant object.

`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.

Verification in the SimBiology GUI

While you are building your model in the SimBiology desktop you can click 

at any time to generate a list of any errors and warnings in the model. The errors and warnings appear in the **Output** pane. Following is an example of the error generated when the reaction rate of a reaction is set to a parameter that you have not defined in SimBiology.



Double-click the error row to move to the location of the error.

Examples

```
modelObj = sbmlimport('radiodecay.xml');
verify(modelObj);
```

See Also

`sbiolasterror`, `sbiolastwarning`

5

Properties — By Category

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
Parameters (p. 5-8)	Properties for parameter objects
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
SimData (p. 5-12)	Properties for SimData objects
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
Variant (p. 5-14)	Properties for variant objects
Using Object Properties (p. 5-17)	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
`Tag`	Specify label for SimBiology object
`Type`	Display top-level SimBiology object type
`UserData`	Specify data to associate with object

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
`Tag`	Specify label for SimBiology object
`Type`	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
`Type`	Display top-level SimBiology object type

Events

Properties for event objects

`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
`Type`	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
`Tag`	Specify label for SimBiology object
`Type`	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
`Tag`	Specify label for SimBiology object
`Type`	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
`Type`	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
`Tag`	Specify label for SimBiology object
`Type`	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
`Type`	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
`Type`	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
`Tag`	Specify label for SimBiology object
`Type`	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
`Tag`	Specify label for SimBiology object

`Type`	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
`Tag`	Specify label for SimBiology object
`Type`	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

`Tag`	Specify label for SimBiology object
`Type`	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. 5-17)	Use either MATLAB functions or object dot notation to enter or change property values
Retrieving Property Values (p. 5-17)	Use either MATLAB functions or object dot notation to get property values
Help for Objects, Methods, and Properties (p. 5-18)	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.
`sbiohelp('MethodName')`	Display method information.
`sbiohelp('PropertyName')`	Display property information.

6

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 i^{th} 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

Example

This example shows how to change `AbsoluteTolerance`.

1 Retrieve the `configset` object from the `modelObj`.

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

2 Change the `AbsoluteTolerance` to `1e-8`.

```
set(configsetObj.SolverOptions, 'AbsoluteTolerance', 1.0e-8);
get(configsetObj.SolverOptions, '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 `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 be `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, variant
Data type	`boolean`
Data values	`true` or `false`. Default value for events, reactions, and rules is `true`. For default `configset` object default is `true`, for added configset object default is `false`. For variants, default is `false`.
Access	Read/Write

Example

1 Create a model object.

```
modelObj = sbiomodel ('my_model');
```

2 Add 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 `Active` property to `'false'` and verify.

```
set (reactionObj, 'Active', false);
get (reactionObj, 'Active')
```

MATLAB returns

```
ans =

0
```

See Also

Methods — `addreaction`, `addrule`, `setactiveconfigset`, `addconfigset`

Objects — `Event object`, `Reaction object`, `Rule object`, `Variant object`

Annotation

Purpose

Store link to URL or file

Description

The `Annotation` property stores URL or filename 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

Example

1 Create a model object

```
modelObj = sbiomodel ('my_model');
```

2 Set annotation for model object

```
set (modelObj, 'annotation', 'www.reactome.org')
```

3 Verify the assignment.

```
get (modelObj, 'annotation')
```

MATLAB returns

```
ans =

www.reactome.org
```

See Also

`addkineticlaw`, `addparameter`, `addreaction`, `addrule`, `addspecies`, `sbiomodel`,`sbioroot`, `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. In SimBiology, all species are state variables regardless of `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 dexamethasone (`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 SimBiology as

```
dex = 0.001
```

- Modeling the role of nucleotides (for example, GTP, ATP, cAMP) and cofactors (for example, Ca^{++}, NAD^{+}, 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

Example

1 Create a model object

```
modelObj = sbiomodel ('my_model');
```

2 Add a species object and verify that boundary condition property setting is `'false'` or `0`.

```
speciesObj = addspecies(modelObj, 'glucose');
get(speciesObj, 'BoundaryCondition')
```

MATLAB returns

```
ans =

     0
```

3 Set 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

Note `BuiltInKineticLaws` produces a warning and will be removed in a future version. Use `BuiltInLibrary` instead.

Description

`BuiltInKineticLaws` is a SimBiology root object property showing all abstract kinetic laws that are shipped with SimBiology. 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');
```

You cannot add, modify, or delete `BuiltInKineticLaws`.

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

Characteristics

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`

MATLAB functions `get` and `set`

Purpose

Library of built-in components

Description

`BuiltInLibrary` is a SimBiology root object property containing all built-in components of unit, 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	`BuiltInLibrary` property
Data type	unit objects
Data values	units
Access	Read-only

- `UnitPrefixes`

Applies to	`BuiltInLibrary` property
Data type	unit prefix objects
Data values	unit prefixes
Access	Read-only

- `KineticLaws`

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

Examples

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

Functions — `sbioaddtolibrary`, `sbioremovefromlibrary` `sbioroot`, `sbiounit`, `sbiounitprefix`

Properties — `UserDefinedLibrary`

BuiltInUnitPrefixes

Purpose

Contain built-in unit prefixes

Note `BuiltInUnitPrefixes` produces a warning and will be removed in a future version. Use `BuiltInLibrary` instead.

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. Both methods are illustrated in the examples below.

You cannot add, modify, or delete `BuiltInUnitsPrefixes`.

Characteristics

Applies to	Object: root
Data type	`char string`
Data values	Valid units
Access	Read-only

See Also

`BuiltInLibrary`

MATLAB functions `get` and `set`.

Purpose

Contain built-in units

Note `BuiltInUnits` produces a warning and will be removed in a future version. 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. Both methods are illustrated in the examples below.

You cannot add, modify, or delete `BuiltInUnits`.

Characteristics

Applies to	Object: root
Data type	`char string`
Data values	Valid units.
Access	Read-only

See Also

`BuiltInLibrary`

Capacity

Purpose

Compartment capacity

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 compartment capacity using rules or events. 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. Default value is `1`.
Access	Read/Write

Example

Add a compartment to a model and set the capacity of the compartment.

1 Create a model object with named `my_model`.

```
modelObj = sbiomodel ('comp_model');
```

2 Add the compartment object with the name `nucleus` and with capacity `0.5`.

```
compartmentObj = addcompartment(modelObj, 'nucleus', 0.5);
```

See Also

Methods — `addcompartmentaddspecies`

Properties — `ConstantCapacity`, `CapacityUnits`

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 object named `my_model`.

```
modelObj = sbiomodel ('my_model');
```

2 Add a compartment object with the name `cytoplasm` and capacity `0.5`

```
compObj = addcompartment (modelObj, 'cytoplasm', 0.5);
```

3 Set the `CapacityUnits` to `femtoliter`, and verify.

```
set (compObj,'CapacityUnits', 'femtoliter');
get (compObj,'CapacityUnits')
```

MATLAB returns

```
ans =

femtoliter
```

See Also

Functions — `sbioaddtolibrary`, `sbioshowunits`, `sbioconvertunits`

Properties — `InitialAmount`

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, below.

You can add a compartment object using the method `addcompartment`.

Characteristics

Applies to	Object: model, compartment
Data type	Array of compartment objects
Data values	Compartment object, default is `[]`
Access	Read-only

Examples

1 Create a model object (`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.

Property Summary

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

Characteristics

Applies to	Object: `configset` object
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

MATLAB functions `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 SimBiology uses 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 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

`Multiplier`, `Offset`, `sbiounit`

MATLAB functions `get` and `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 example of modeling species as constant amounts:

Modeling the role of nucleotides (GTP, ATP, cAMP) and cofactors (Ca^{++}, NAD^{+}, 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

Example

1 Create a model object with name `my_model`.

```
modelObj = sbiomodel ('my_model');
```

2 Add a species object and verify that the `ConstantAmount` property setting is `'false'` or `0`

```
speciesObj = addspecies (modelObj, 'glucose');
get (speciesObj, 'ConstantAmount')
```

MATLAB returns

```
             ans =

        0
```

3 Set constant amount to `'true'` and verify

```
set (speciesObj, 'ConstantAmount', true);
get (speciesObj, 'ConstantAmount')
```

MATLAB returns

```
ans =

     1
```

See Also

`addspecies`, `BoundaryCondition`

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

Example

Add a compartment to a model and check the `ConstantCapacity` property of the compartment.

1 Create a model object with named `my_model`.

```
modelObj = sbiomodel ('comp_model');
```

2 Add the compartment object with the name `nucleus` and with capacity `0.5`.

```
compartmentObj = addcompartment(modelObj, 'nucleus', 0.5);
```

3 Display the `ConstantCapacity` property.

```
get(compartmentObj, 'ConstantCapacity')

ans =

     1
```

See Also

Methods — `addcompartment`

Properties — `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:

$$Aspartic\ \text{acid} \xrightarrow{\text{aspartate kinase}} \beta - Aspartylphosphate$$

$$\beta - Aspartylphosphate \longrightarrow Threonine$$

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`

Data values	`true` or `false`. Default value is `'true'`.
Access	Read/Write

Example

1 Create a model object.

```
modelObj = sbiomodel ('my_model');
```

2 Add parameter object.

```
parameterObj = addparameter (modelObj, 'kf');
```

3 Change the `ConstantValue` property of the parameter object from default (`true`) 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

`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 `[]`.
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:
   1                 species      A                 InitialAmount
   2                 species      B                 InitialAmount
```

3 Append data to the `Content` property.

```
addcontent(variantObj, {'species', 'C', 'InitialAmount', 15});

SimBiology Variant - v1 (inactive)

   ContentIndex:     Type:        Name:             Property:
   1                 species      A                 InitialAmount
   2                 species      B                 InitialAmount
   3                 species      C                 InitialAmount
```

4 Remove a species from the `Content` property.

```
rmcontent(variantObj, 3);
```

5 Replace the data in the `Content` property.

```
set(variantObj, 'Content', {'species', 'C', 'InitialAmount', 15});
```

See Also

`sbiovariant`, `addcontent`, `rmcontent`

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 x 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 `[]`.
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

Applies to	Object: SimData
Data type	`struct`
Data values	Default value for each field is `0`.
Access	Read-only

See Also

`StopTimeType`, `StopTime`

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:

Type	Fields

Species	`Type: species`
	`Name:`
	`Compartment:`
	`Units:`

Type	Fields

Parameter	`Type: parameter`
	`Name:`
	`Reaction: <name of reaction that a parameter is scoped to,`
	`or '' if parameter is scoped to model>`
	`Units:`

Sensitivity	`Type: sensitivity`
	`Name: <for example: d[x]/d[y]_0>`
	`OutputType: <The type of the sensitivity output,`
	`either `species' or `parameter'>`
	`OutputName: <The name of the sensitivity output>`
	`OutputQualifier: <The compartment or reaction for`
	`the sensitivity output, for`
	`species or parameters, respectively>`
	`InputType: <The type of the sensitivity input,`
	`either `species' or `parameter'>`
	`InputName: <The name of the sensitivity input>`
	`InputQualifier: <The compartment or reaction for`
	`the sensitivity input, for`
	`species or parameters, respectively>`
	`Units:`

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 in SimData object

Description

The `DataNames` property holds the names labeling the columns of the data matrix in the `Data` property. The property contains an `nx1` array of strings. SimBiology 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

`StopTimeType`, `StopTime`

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

`DimensionalAnalysis`, `CompileOptionsgetconfigset`, `sbiosimulate`

MATLAB functions `get` and `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`, SimBiology 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

Example

Shows how to retrieve and set `DimensionalAnalysis` from the default `true` to `false` in the default configuration set in a model object.

1 Import a model.

```
modelObj = sbmlimport('oscillator')


SimBiology Model - Oscillator

   Model Components:
     Models:            0
     Parameters:        0
     Reactions:         42
     Rules:             0
     Species:           23
```

2 Retrieve the `configset` object of the model object.

```
configsetObj = 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
```

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

`getconfigset`, `sbiosimulate`

MATLAB functions `get` and `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 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; default is `3e-2`
Access	Read/Write

Example

Shows how to change `ErrorTolerance` 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 `ErrorTolerance` to `1e-8`.

```
set(configsetObj.SolverOptions, 'ErrorTolerance', 5.0e-2);
get(configsetObj.SolverOptions, 'ErrorTolerance')


ans =

  5.000000e-002
```

See Also

LogDecimation, RandomState

Purpose

Event expression

Description

Property of event object that defines what occurs when the event is triggered. Specify 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 SimBiology Evaluates Events" in the SimBiology User's Guide. For examples of event functions see "Specifying Event Functions" in the SimBiology User's Guide.

Characteristics

Applies to	Object: event
Data type	cell array of strings
Data values	`EventFcn` strings `''`
Access	Read/Write

Examples

1 Create a model object, and then add an event object.

```
modelObj = sbmlimport('oscillator');
eventObj = addevent(modelObj, 'time>= 5', 'OpC = 200');
```

2 Set the `EventFcns` property of the event object.

```
set(eventObj, 'EventFcns', {'pA = OpA','mA = pol'});
```

3 Get the `EventFcns` property.

```
get(eventObj, 'EventFcns')
```

See Also

`Event object`, `Trigger`

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 “Events” in the SimBiology User’s Guide for more information.

Add an event to a `Model` object with the method `addevent` method and remove an event with the `deletemethod`. 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, Default is empty (`[]`).
Access	Read-only

Examples

1 Create a model object, and then add an event object.

```
modelObj = sbmlimport('oscillator')
eventObj = addevent(modelObj, 'time>= 5', 'OpC = 200');
```

2 Get a list of properties for an event object.

```
get(modelObj.Events(1));
```

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

`Model object`, `Event object`, `EventFcns`, `Trigger`

Exponent

Purpose

Exponent value of unit prefix

Description

Exponent shows the value of `10^Exponent` that defines the numerical value of the unit prefix*Name*. 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	Object: Unit prefix
Data type	`double`
Data values	Real number. Default is `0`
Access	Read/Write

Examples

This example shows you how to create a user-defined unitprefix, add it to the user-defined library, and query the `Exponent` property.

1 Create a unitprefix.

```
unitprefixObj1 = sbiounitprefix('peta', 15);
```

2 Add the unitprefix to the user-defined library.

```
sbioaddtolibrary(unitprefixObj1);
```

3 Query the `Exponent` property.

```
get(unitprefixObj1, 'Exponent')

ans =

    15
```

See Also

`sbioaddtolibrary`, `sbiounitprefix`,`UnitPrefix object`

MATLAB functions `get` and `set`.

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 builtin 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 `ParameterVariables`property 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 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.

Expression

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 i^{th} 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 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: kineticlaw, abstract 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 `reactionObj`is 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, 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

Abstract and kinetic law object properties: `SpeciesVariables`, `ParameterVariables`

Kinetic law object properties: `KineticLawName`, `Parameters`, `SpeciesVariableNames`, `ParameterVariableNames`

Reaction object property: `ReactionRate`

Functions: `sbioaddtolibrary`, `sbiowhos`

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

Example

Add a species to a model and set the initial amount of the species.

1 Create a model object with named `my_model`.

```
modelObj = sbiomodel ('my_model');
```

2 Add the species object with the name `glucose`.

```
speciesObj = addspecies (modelObj, 'glucose');
```

3 Set the initial amount to `100` and verify.

```
set (speciesObj, 'InitialAmount',100);
get (speciesObj, 'InitialAmount')
```

MATLAB returns

```
ans =

   100
```

See Also

`addspecies`, `InitialAmountUnits`

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 builtin units. To get a list of the defined units use the `sbioshowunits` function. If `InitialAmountUnits` changes from one unit definition to another, the `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`^{2} then species must be `amount/meter`^{2} 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 = `''` (empty)
Access	Read/Write

Example

1 Create a model object named `my_model`.

```
modelObj = sbiomodel ('my_model');
compObj = addcompartment(modelObj, 'cell');
```

2 Add a species object with the name `glucose`.

```
speciesObj = addspecies (compObj, 'glucose');
```

3 Set the initial amount to `100`, `InitialAmountUnits` to `molecule`, and verify.

```
set (speciesObj,'InitialAmountUnits','molecule');
get (speciesObj,'InitialAmountUnits')
```

MATLAB returns

```
ans =

molecule
```

See Also

DefaultSpeciesDimension, InitialAmount, sbioshowunits, sbioconvertunits, sbioregisterunit

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, 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');
```

3 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

Kinetic law object properties: `KineticLawName`, `Parameters`, `SpeciesVariableNames`, `ParameterVariableNames`

Reaction object property: `ReactionRate`

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 builtin 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 `KineticLawName` of `kineticlawObj`

```
get (kineticlawObj, 'KineticLawName')
```

MATLAB returns

```
ans =
```

```
Henri-Michaelis-Menten
```

See Also

Abstract and kinetic law object properties: `Expression`, `SpeciesVariables`, `ParameterVariables`

Kinetic law object properties: `Parameters`, `SpeciesVariableNames`, `ParameterVariableNames`

Reaction object property: `ReactionRate`

Functions: `sbioaddtolibrary`, `sbiowhos`

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

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 =
```

```
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 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

Example

Shows how to change `MaxIterations` settings.

1 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);
```

```
get(configsetObj.SolverOptions, 'MaxIterations')

ans =

  25
```

See Also

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

Applies to	Object: `SolverOptions`
Data type	`Positive scalar`
Data values	`{0.1*abs(t0-tf)}` default is `[]`
Access	Read/Write

See Also

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.

Characteristics

Applies to	Object: SimData
Data type	`string`
Data values	Default value is `''`.
Access	Read-only

See Also

`Data`, `DataInfo`

Purpose

Contain all model objects

Note The `Models` property will be removed in a future version. Submodels will not be supported in future releases. Use the function `sbioupdate` to convert 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	Objects: model, root
Data type	Array of model objects
Data values	Model object, Default is empty (`[]`).
Access	Read-only

See Also

`sbiomodel`, `sbioupdate`

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	Object: Unit
Data type	`double`
Data values	Non-zero real number. Default value is 1.
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 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
```

See Also

`Composition`, `Offset`, `sbiounit`

MATLAB functions `get` and `set`.

Name

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 non-unique species names if the species are in different compartments, and non-unique parameter names if the parameters are in different kinetic laws or at different levels. Note that having non-unique 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.

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 :

- Models names cannot be empty.
- Parameters 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 square brackets . For example, enclose `[DNA polymerase+]` within 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 compartments names cannot be empty and note the following reserved words, characters and constraints:

- 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

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

1 Create a model object with the name `my_model`.

```
modelObj = sbiomodel ('my_model');
```

2 Add a reaction object to the model object. Note the use of square brackets because the names are not valid MATLAB variable names.

```
reactionObj = addreaction(modelObj, '[Aspartic acid] -> [beta-Aspartyl-PO4]')
```

MATLAB returns

```
SimBiology Reaction Array

Index:    Reaction:
  1       [Aspartic acid] -> [beta-Aspartyl-PO4]
```

3 Set reaction `Name` and verify

```
set (reactionObj, 'Name', 'Aspartate kinase reaction');
get (reactionObj, 'Name')
```

MATLAB returns

```
ans =

  Aspartate kinase reaction
```

See Also

Functions — `sbiomodel`, `sbiounit`, `sbiounitprefix`

Methods — `addcompartment`, `addkineticlaw`, `addmodel`, `addparameter`, `addreaction`, `addrule`, `addspecies`

Purpose

Specify normalization type for sensitivity analysis

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.

$$\frac{dx(t)}{dk}$$

- `'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`

Notes

Purpose

HTML text describing SimBiology object

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, unit prefix
Data type	`char string`
Data values	Any `char string`
Access	Read/Write

Example

1 Create a model object.

```
modelObj = sbiomodel ('my_model');
```

2 Write notes for the model object.

```
set (modelObj, 'notes', '09/01/05 experimental data')
```

3 Verify the assignment

```
get (modelObj, 'notes')
```

MATLAB returns

```
ans =

09/01/05 experimental data
```

See Also

`addkineticlaw`, `addmodel`, `addparameter`, `addreaction`, `addrule`, `addspecies`, `sbiomodel`, `sbiounit`, `sbiounitprefix`

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

Applies to	Object: Unit
Data type	`double`
Data values	Real number. Default is `0`
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 library.

1 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);
```

2 Add the unit to the user-defined library.

```
sbioaddtolibrary(unitObj);
```

3 Query the `Offset` property.

```
get(unitObj, 'Offset')

ans =

32
```

See Also

`Composition`, `Multiplier`, `sbioaddtolibrary`, `sbioshowunits`, `sbiounit`.

MATLAB functions `get` and `set`.

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 ompartment object, default is `[]`
Access	Read-only

Examples

1 Create a model object (`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 it's components:

```
SimBiology Compartment - mitochondrion
```

```
Compartment Components:
  Capacity:          1
  CapacityUnits:
  Compartments:      1
  ConstantCapacity:  true
  Owner:
  Species:           0
```

See Also

Parent, Compartments

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, SimBiology 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	parameter object or array of parameter objects
Data values	Parameter object array. Default is `[]`.
Access	Read/Write

Examples

This example shows how to set `ParameterInputFactors` for sensitivity analysis.

1 Import the radio decay model from SimBiology demos.

```
modelObj  = sbmlimport('radiodecay');
```

2 Retrieve the configuration set object from `modelObj`.

```
configsetObj = getconfigset(modelObj);
```

3 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

SimBiology function `sbioselect`

SimBiology properties `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

Example

1 Create a model object, 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:    Name:    Value:    ValueUnits:
   1         K2       1
```

See Also

`addparameter`, `delete`, `sbioparameter`

MATLAB functions `get` and `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 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

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 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

Reaction object property: `ReactionRate`

Abstract kinetic law object and kinetic law object properties: `Expression`, `SpeciesVariables`, `ParameterVariables`

Kinetic law object property: `SpeciesVariableNames`

Method: `setparameter`

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, 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.

```
get (kineticlawObj, 'ParameterVariables')
```

MATLAB returns

```
ans =

    'Vm' 'Km'
```

See Also

Reaction object property: `ReactionRate`

Abstract kinetic law object and kinetic law object properties: `Expression`, `SpeciesVariables`

Kinetic law object property: `SpeciesVariableNames`, `ParameterVariableNames`

Method: `setparameter`

MATLAB function `set`

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 • root object upon addition to library
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

Object	Parent
variant	model object or [] (empty)
unit and unit prefixes	• [] (empty) until added to library • root object upon addition to library

Characteristics

Applies to	Objects: abstract kinetic law, compartment, event, kinetic law, model, parameter, reaction, rule, species, variant, unit, unit prefix
Data type	Object
Data values	SimBiology component object or empty [].
Access	Read-only

See Also

`sbiomodel`, `addkineticlaw`, `addmodel`, `addparameter`, `addreaction`

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 `[]`.
Access	Read-only

Example

1 Create a model object

```
modelObj = sbiomodel ('my_model');
```

2 Add reaction objects

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

3 Verify assignment.

```
productsObj = get(reactionObj, 'Products')
```

MATLAB returns

```
SimBiology Species Array

Index:  Compartment:  Name:  InitialAmount: InitialAmountUnits:
```

```
    1        unnamed        c        0
    2        unnamed        d        0
```

See Also

addkineticlaw, addspecies, addproduct, 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 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 resets the state at startup. The default value of `RandomState` is `[]`.

Characteristics

Applies to	Object: `SolverOptions` for `SSA`, `expltau`, `impltau`
Data type	`int`
Data values	Default is `[]`.
Access	Read/Write

Example

Shows how to change `RandomState` 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 `Randomstate` to `5`.

```
set(configsetObj.SolverOptions, 'RandomState', 5);
```

```
get(configsetObj.SolverOptions, 'RandomState'))

ans =

  5
```

See Also

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

Applies to	Objects: reaction
Data type	Species object or array of species objects
Data values	Species objects, default is `[]`
Access	Read-only

Example

1 Create a model object

```
modelObj = sbiomodel ('my_model');
```

2 Add reaction objects

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

3 View the reactants for `reactionObj`.

```
get(reactionObj, 'Reactants')
```

MATLAB returns

```
SimBiology Species Array

Index:  Compartment:  Name:  InitialAmount: InitialAmountUnits:
 1       unnamed        a        0
```

```
     2        unnamed         b         0
```

See Also

addreaction, addspecies, addreactant, rmreactant

Purpose

Reaction 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 `Reaction` property is set.

Characteristics

Applies to	Object: reaction
Data type	`char string`
Data values	Valid reaction string, default is `''`
Access	Read/Write

Example

1 Create a model object, 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

`sbioreaction`, `addreaction`

ReactionRate

Purpose

Reaction rate equation in reaction object

Description

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 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.

Once you have specified the `ReactionRate` without `KineticLaw`, if 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 `''`
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, 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 a names `Vm_d, 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, 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

`sbioreaction`, `addreaction`, `sbioparameter`, `addparameter`, `Reversible`

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

Applies to	Objects: model
Data type	Array of reaction objects
Data values	Reaction object
Access	Read-only

Example

1 Create a model object, then add a reaction object

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

2 Verify that the reactions property records the input

```
get (modelObj, 'Reactions')
```

MATLAB returns

```
SimBiology Reaction Array

 Index:    Reaction:
   1       a + b -> c + d
```

See Also

`sbioreaction`, `addreaction`, `delete`

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.

`RelativeTolerancet` is a property of `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 i^{th} state vector `y`. Simulation converges at that time step if e_i satisfies the following equation:

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

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.

Characteristics

Applies to	Object: `SolverOptions`
Data type	`double`

Data values	>0, <1; default is `1e-3`.
Access	Read/Write

Example

Shows how to change `AbsoluteTolerance`.

1 Retrieve the `configset` object from the `modelObj`.

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

2 Change the `AbsoluteTolerance` to `1e-8`.

```
set(configsetObj.SolverOptions, 'RelativeTolerance', 1.0e-6);
get(configsetObj.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

Example

Create a model, add a reaction, and assign the expression for the reaction rate equation.

1 Create model object, 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`) with names `Kf, 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

sbioreaction, addreaction, addparameter, addreactant, ParameterVariableNames, ReactionRate

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, then add a reaction object

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

2 Add a rule

```
ruleObj = addrule(modelObj, '10-a+b')
```

MATLAB returns

```
SimBiology Rule Array

Index:    RuleType:    Rule:
1         algebraic    10-a+b
```

See Also

`addrule`, `delete`, `sbiorule`

RuleType

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`, and `sbiorule`

The rule types defined are as follows:

- **`algebraic`** — Algebraic rules are evaluated continuously during a simulation. An algebraic rule takes the form `0 = Expression` and the rule is specified as the `Expression`. For example, you could write a mass conservation expression such as `species_total = species1 + species2` where `species_total` is the independent variable, type the rule as follows: `species1 + species2 - species_total`
- **`initialAssignment`** — `initialAssignment` rules are evaluated once at the beginning of a simulation. `initialAssignment` rules are expressed as `Variable = Expression`. For example you could write an `initialAssignment` rule to set the amount of `species1` to be proportional to `species2`. Type the rule as follows: `species1 = k/species2`
- **`repeatedAssignment`** — `repeatedAssignment` rules are evaluated at every time-step during a simulation. `repeatedAssignment` rules are expressed as `Variable = Expression`. For example, you could use the rule to specify the amount of `species1` to always be proportional to `species2`. Type the rule as follows: `species1 = k/species2`
- **`rate`** — `rate` rules are evaluated continuously during a simulation. Rate rules are determined by `dVariable/dt = Expression` which is expressed in SimBiology as `Variable = Expression`. For

example, to define the rate of change in the quantity of `species3` (`d(species3)/dt`). Type the rule as follows: `species3 = k * (species1 + species2)`

One example case for a rate rule is when `Species1` is at the boundary of the system, but the rate of input of `species1` to the system can be determined by a rate rule.

Note If you use a parameter in a rule, remember to set the scope of the parameter to the model. Further, if you are using an `algebraic`, `repeatedAssignment`, or `rate` rule to vary the value of a parameter during the simulation, set the `ConstantValue` property of the parameter to false. You can use the `initialAssignment` rule on a constant parameter, that is, a parameter that has the `ConstantValue` property equal to `true`.

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 `initialAssigment` 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.

RuleType

Characteristics

Applies to	Object: rule
Data type	`char string`
Data values	`'algebraic'`, `'assignment'`, `'rate'`. Default value is `'assignment'`.
Access	Read/write

Example

1 Create a model object, 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 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

sbiorule, addrule, delete

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 **rule** 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

Example

1 Create a model object, then add a reaction object

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

2 Add a rule

```
ruleobj = addrule(modelObj, '10-a+b')
```

MATLAB returns

```
SimBiology Rule Array

Index:    RuleType:    Rule:
 1        algebraic    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` are rarely empty, since these fields are populated after simulation.

Access	Read-only

See Also

`StopTimeType`, `StopTime`

RuntimeOptions

Purpose

Options for logged species

Description

The `RuntimeOptions` property holds options for species that will be logged during the simulation run. The runtime options object can be accessed through this property.

The `LogDecimation` property of the configuration set object defines how often data is logged.

Property Summary

`StatesToLog`	Specify species data recorded
`Type`	Display top-level SimBiology object type

Characteristics

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

Example

1 Create a model object and retrieve its configuration set.

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

2 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" 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')

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 6-116.

When sensitivity analysis is enabled, the following command

```
[t,x,names] = sbiosimulate(modelObj)
```

returns `[t,x,names]`, where

- `t` is a `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 a `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 facto
  ```

  A SimBiology state includes species and non-constant 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.

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.

SensitivityAnalysisOptions

Property Summary

`Normalization`	Specify normalization type for sensitivity analysis
`ParameterInputFactors`	Specify parameter input factors for sensitivity analysis
`SpeciesInputFactors`	Specify species inputs for sensitivity analysis
`SpeciesOutputs`	Specify species outputs for sensitivity analysis

Characteristics

Applies to	Object: configuration set object
Data type	Object
Data values	`SensitivityAnalysisOptions` properties as summarized in “Property Summary” on page 6-116 .
Access	Read-only

Examples

This example shows how to set `SensitivityAnalysisOptions`.

1 Import the radio decay model from SimBiology demos.

```
modelObj  = sbmlimport('radiodecay');
```

2 Retrieve the `configset` object from the `modelObj`.

```
configsetObj = getconfigset(modelObj);
```

3 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
```

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 for more information.

```
[t,x,names] = sbiosimulate(modelObj);
```

7 Display `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`.

```
x
```

SimBiology 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 solver options in the `configset` object. Changing the property `SolverType` changes the options specified in the `SolverOptions` object.

Properties of `SolverOptions` are summarized in the property summary on this page.

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
`Type`	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

Example

Illustrates 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 let 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”.

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

Example

1 Retrieve the configset object from the modelObj.

```
modelObj  = sbiomodel('cell');
configsetObj = 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 `ode45`.

```
set(configsetObj, 'SolverType', 'ode45')
configsetObj

  Configuration Settings - default (active)
    SolverType:           ode45
    StopTime:             10.000000

  SolverOptions:
    AbsoluteTolerance:    1.000000e-006
    RelativeTolerance:    1.000000e-003

  RuntimeOptions:
    StatesToLog:          all

  CompileOptions:
    UnitConversion:       true
    DimensionalAnalysis:  true
```

See Also

`getconfigset`

MATLAB function `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 *`compartmentName.speciesName`*, 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 *not* 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 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.

SimBiology 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, SimBiology 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 `[]`.
Access	Read/Write

Examples

This example shows how to set `SpeciesInputFactors` for sensitivity analysis.

1. Import the radio decay model from 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

SimBiology function `sbioselect`

SimBiology properties `SensitivityAnalysis`, `SensitivityAnalysisOptions`, `ParameterInputFactors`

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.

SimBiology 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, SimBiology returns the computed sensitivities of the species specified in `SpeciesOutputs`. 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 `[]`.
Access	Read/Write

Examples

This example shows how to set `SpeciesOutputs` for sensitivity analysis.

1 Import the radio decay model from 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

SimBiology function `sbioselect`

SimBiology properties `ParameterInputFactors`, `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 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

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');
```

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

Reaction object property: `ReactionRate`

Abstract kinetic law object and kinetic law object properties: `Expression`, `SpeciesVariables`, `ParameterVariables`

Kinetic law object property: `ParameterVariableNames`

Method: `setparameter`

Purpose

Species in abstract kinetic law

Description

Property showing 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.

Example

Create a model, add a reaction, and assign the `SpeciesVariableNames` for the reaction rate equation.

1 Create a model object, 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

```
ans =

    'S'
```

See Also

Reaction object property: `ReactionRate`

Abstract kinetic law object and kinetic law object properties: `Expression`, `ParameterVariables`

Kinetic law object property: `ParameterVariableNames`, `SpeciesVariableNames`

Method: `setparameter`

MATLAB function `set`

Purpose

Specify 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

Example

Illustrates 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 the `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

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` functions. 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 only support 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

Example

1 Create a reaction object

```
reactionObj = sbioreaction('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

`sbioreaction`, `addreaction`, `addproduct`, `addreactant`, `rmproduct`, `rmreactant`, `Reaction`

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	Object: `configset`
Data type	`double`
Data values	Enter a positive number. Default is `10`.
Access	Read/Write

Example

1 Retrieve the `configset` object from the `modelObj`.

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

2 Configure the `StopTime` to `20`.

```
set(configsetObj, 'StopTime', 20)
get(configsetObj, 'StopTime')

ans =

    20
```

See Also

`StopTimeType`, `TimeUnits`

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

Example

1 Retrieve the `configset` object from the `modelObj`.

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

2 Configure the `StopTimeType` to `approxWallTime`.

```
set(configsetObj, 'StopTimeType', 'approxWallTime');
get(configsetObj, 'StopTimeType')

ans =

approxWallTime
```

See Also

`StopTime`, `StatesToLog`, `TimeUnits`

MATLAB function `set`

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, species
Data type	`char string`
Data values	Any `char string`
Access	Read/Write

Example

1 Create a model object.

```
modelObj = sbiomodel ('my_model');
```

2 Add reaction object and set Tag property to `'Synthesis Reaction'`.

```
reactionObj = addreaction (modelObj, 'a + b -> c + d');
set (reactionObj, 'Tag', 'Synthesis Reaction')
```

3 Verify `Tag` assignment.

```
get (reactionObj, 'Tag');
```

MATLAB returns

```
ans =

     'Synthesis Reaction'
```

See Also

sbiomodel, sbioabstractkineticlaw, addkineticlaw, addparameter, addreaction, addrule, addspecies, 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 SimBiology handles events see, "How SimBiology Evaluates Events" in the SimBiology User's Guide. For examples of event functions see "Specifying Event Triggers" in the SimBiology User's Guide.

Characteristics

Applies to	Object: event
Data type	String, function handle
Data values	Specify MATLAB expression as string. Default is `''` (None).
Access	Read/Write

Examples

1 Create a model object, and then add an event object.

```
modelObj = sbmlimport('oscillator');
eventObj = addevent(modelObj, 'time>= 5', 'OpC = 200');
```

2 Set the `Trigger` property of the event object.

```
set(eventObj, 'Trigger', '(time >=5) && (speciesA<1000)');
```

3 Get the `Trigger` property.

```
get(eventObj, 'Trigger')
```

See Also

`Event object`, `EventFcns`

Purpose

Show simulation time steps

Description

The `Time` property shows the time points in a simulation.

Characteristics

Applies to	Object: SimData
Data type	`double`
Data values	Vector of doubles.
Access	Read-only

See Also

`StopTimeType`, `StopTime`

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 `seconds`.

Characteristics

Applies to	Object: `configset`
Data type	`string`
Data values	Default value is `second`.
Access	Read-only

See Also

`StopTimeType`, `StopTime`

Purpose

Display top-level SimBiology object type

Description

The `Type` property indicates a SimBiology object type. When you create an object in SimBiology, 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`, `SolverOptions`.
Data type	`char string`
Data values	`abstract_kinetic_law`, `configset`, `compileoptions`, `kineticlaw`, `parameter`, `reaction`, `root`, `rule`, `runtimeoptions`, `sbiomodel`, `species`, `solveroptions`.
Access	Read-only

See Also

`sbiomodel`, `sbioparameter`, `sbioreaction`, `sbioroot`, `sbiorule`, `sbiospecies`

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.

When `UnitConversion` is set to `true`, SimBiology converts the matching physical quantities to one consistent unit system in order to resolve them. This conversion is in preparation for correct simulation, but species amounts are returned in the user-specified units.

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/((molecules/liter)*second)`, `UnitConversion` occurs after `DimensionalAnalysis`.

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 you simulate (`sbiosimulate`).

If `UnitConversion` is set to `false`, SimBiology 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

Example

Shows how to retrieve and set `unitconversion` from the default `true` to `false` in the default configuration set in a model object

1 Import a model.

```
modelObj = sbmlimport('oscillator')


SimBiology Model - Oscillator

   Model Components:
     Models:            0
     Parameters:        0
     Reactions:         42
     Rules:             0
     Species:           23
```

2 Retrieve the `configset` object of the model object.

```
configsetObj = 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:       false
    DimensionalAnalysis:  true
```

3 Retrieve the `CompileOptions` object.

```
optionsObj = get(configsetObj,'CompileOptions')

Compile Settings:

    UnitConversion:       false
    DimensionalAnalysis:  true
```

4 Assign a value of false to `UnitConversion`.

```
 set(optionsObj,'UnitConversion', true)
```

See Also

`getconfigset`, `sbiosimulate`.

MATLAB functions `get` and `set`.

Purpose

Specify data to associate with object

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

`sbiomodel`, `sbioabstractkineticlaw`, `sbioparameter`, `sbioreaction`, `sbioroot`, `sbiorule`, `sbiospecies`, `sbiounit`, `sbiounitprefix`

UserDefinedKineticLaws

Purpose

Contain user-defined kinetic laws

Note `UserDefinedKineticLaws` produces a warning and will be removed in a future version. 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:

```
kineticlawObj = addkineticlaw(reactionObj, 'my_kinetic_law');
```

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.

Characteristics

Applies to	Object: root
Data type	`char string`
Data values	Valid kinetic laws
Access	Read/Write

See Also

Functions — `sbioaddtolibrary`

Properties — `AbstractKineticLaw object`, `UserDefinedLibrary`,

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 law objects
Access	Read-only

Characteristics for `UserDefinedLibrary` 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
Access	Read/Write

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

Functions — `sbioaddtolibrary`, `sbioremovefromlibrary` `sbioroot`, `sbiounit`, `sbiounitprefix`

Properties — `BuiltInLibrary`

UserDefinedUnitPrefixes

Purpose

Contain user-defined unit prefixes

Note `UserDefinedUnitPrefixes` produces a warning and will be removed in a future version. 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
Access	Read/Write

See Also

`sbioaddtolibrary`, `UserDefinedLibrary`, `UnitPrefix object`

Purpose

Contain user-defined units

Note `UserDefinedUnits` produces a warning and will be removed in a future version. 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
Data type	`char string`
Data values	Valid units
Access	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	Object: parameter
Data type	`double`
Data values	Any `double`. Default value is 1.0.
Access	Read/Write

Example

Assign a parameter with value to the model object

1 Create a model object, 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
```

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 builtin units. To get a list of the builtin 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	Object: parameter
Data type	`char string`
Data values	Unit from units library, default is empty `''`
Access	Read/Write

Example

Assign a parameter with value to the model object.

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

```
modelObj = sbiomodel('my_model');
```

2 Add a parameter with `Value` `0.5` , assign it to the model object (`modelObj`).

```
parameterObj1 = addparameter(modelObj, 'K1', 0.5, 'ValueUnits', '1/second')
```

MATLAB returns

```
SimBiology Parameter Array

Index:    Name:    Value:    ValueUnits:
 1         K1       0.5       1/second
```

See Also

`sbioparameter`, `addparameter`, `sbioshowunits`, `sbioconvertunits`

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