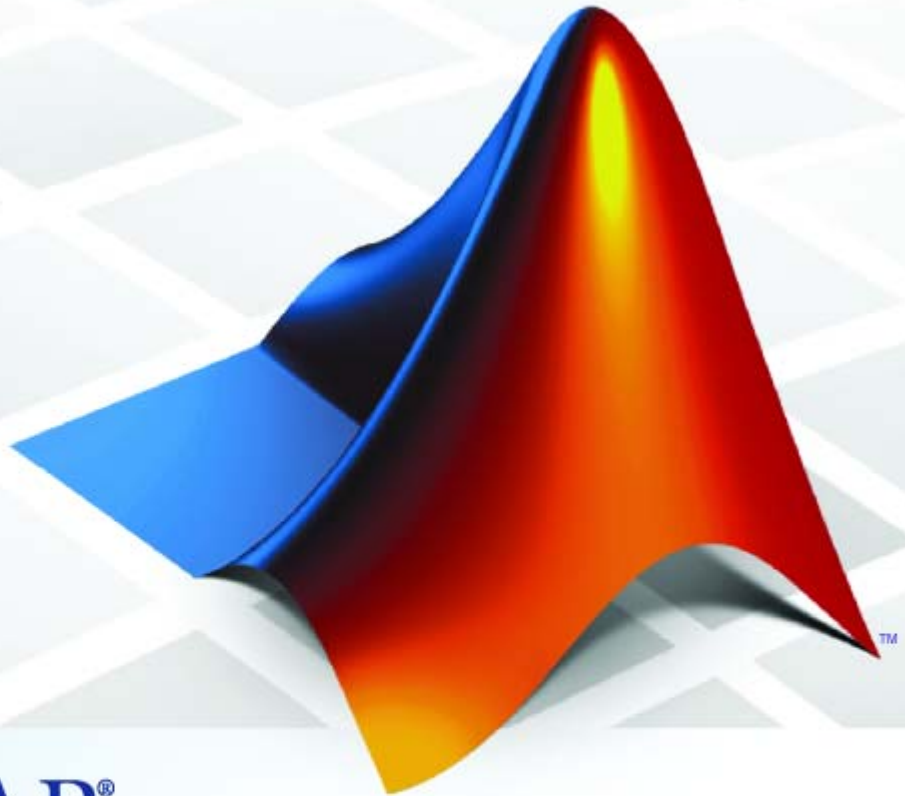


SimBiology[®] 3

Reference



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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+)
March 2008	Online only	Updated for Version 2.3 (Release 2008a)
October 2008	Online only	Updated for Version 2.4 (Release 2008b)
March 2009	Online only	Updated for Version 3.0 (Release 2009a)
September 2009	Online only	Updated for Version 3.1 (Release 2009b)
March 2010	Online only	Updated for Version 3.2 (Release 2010a)

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tools

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Export and import SBML models

Create SimBiology® objects

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Perform unit conversion and create
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<code>sbiounitprefix</code>	Create user-defined unit prefix

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sbioabstractkineticlaw

Purpose Create kinetic law definition

Syntax

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

Arguments

<i>Name</i>	Enter a name for the kinetic law definition. Name must be unique in the user-defined kinetic law library. Name is referenced by <i>kineticlawObj</i> .
<i>Expression</i>	The mathematical expression that defines the kinetic law.

Description

abstkineticlawObj = sbioabstractkineticlaw('Name') creates an abstract kinetic law object, with the name *Name* and returns it to *abstkineticlawObj*. Use the abstract kinetic law object to specify a *kinetic law definition*.

The *kinetic law definition* provides a mechanism for applying a specific rate law to multiple reactions. It acts as a mapping template for the reaction rate. The kinetic law definition 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 the kinetic law definition, it must be added to the user-defined library with the *sbioaddtolibrary* function. To get the kinetic law definitions in the user-defined library, use the command `get(sbioroot, 'UserDefinedKineticLaws')`.

abstkineticlawObj = sbioabstractkineticlaw('Name', 'Expression') constructs a SimBiology abstract kinetic law object, *abstkineticlawObj*

with the name '*Name*' and with the expression '*Expression*' and returns it to *abstkineticlawObj*.

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

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

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 kinetic law definition
Parent	Indicate parent object
SpeciesVariables	Species in abstract kinetic law

sbioabstractkineticlaw

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

Examples

- 1 Create a kinetic law definition.

```
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 kinetic law definition to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

`sbioaddtolibrary` adds the kinetic law definition 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 kinetic law definition when defining a reaction's kinetic law.

```
modelObj = sbiomodel('cell');  
reactionObj = addreaction(modelObj, 'A + B <-> B + C');  
kineticlawObj = addkineticlaw(reactionObj, 'ex_myLaw1');
```

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

See Also

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

sbioaccelerate

Purpose Prepare model object for accelerated simulations

Syntax

```
sbioaccelerate(modelObj)
sbioaccelerate(modelObj, configsetObj)
sbioaccelerate(modelObj, variantObj)
sbioaccelerate(modelObj, doseObj)
sbioaccelerate(modelObj, configsetObj, variantObj)
sbioaccelerate(modelObj, configsetObj, doseObj)
sbioaccelerate(modelObj, configsetObj, variantObj, doseObj)
```

Description Use the same arguments in `sbioaccelerate` that you will use in the subsequent call to `sbiosimulate`.

`sbioaccelerate(modelObj)` prepares a model object (`modelObj`) for accelerated simulation using its active configset, active variants and active doses. A SimBiology model can contain multiple configsets with one being active at any given time. The active configset contains the settings that will be used to prepare the model for acceleration.

`sbioaccelerate(modelObj, configsetObj)` uses the configset `configsetObj`. A configset object stores simulation specific information.

`sbioaccelerate(modelObj, variantObj)` uses the variant object or array of variant objects `variantObj`. A variant object's settings supersede model property-values.

`sbioaccelerate(modelObj, doseObj)` simulates `modelObj` using the dose object or array of dose objects `doseObj`. A SimBiology Dose object defines additions that are made to species amounts or parameter values.

`sbioaccelerate(modelObj, configsetObj, variantObj)`,
`sbioaccelerate(modelObj, configsetObj, doseObj)` uses the configset `configsetObj` and variant object or variant array `variantObj` or dose object or dose array `doseObj`. Note if the third argument is empty it is assumed to be `variantObj`.

`sbioaccelerate(modelObj, configsetObj, variantObj, doseObj)`

Input Arguments

modelObj

SimBiology model object.

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.

doseObj

Specify the dose object to apply to the model during the simulation. For more information about dose objects, see `ScheduleDose` object and `RepeatDose` object.

Examples

This example shows how to prepare a model for accelerated simulation.

```
% Create a SimBiology model from an SBML file.
m = sbmlimport('lotka.xml');

% Prepare the model for accelerated simulation.
sbioaccelerate(m);

% Simulate the model for different initial amounts of x.
x = sbioselect(m, 'type', 'species', 'name', 'x');
for i=1:10
    x.initialAmount = i;
    sd(i) = sbiosimulate(m);
end

% Plot the results.
sbioplot(sd);
```

sbioaccelerate

See Also

`sbiosimulate`

Purpose Add to user-defined library

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

Arguments

<i>abstkineticlawObj</i>	Specify the abstract kinetic law object that holds the kinetic law definition. The Name of the kinetic law must be unique in the user-defined kinetic law library. Name is referenced by <i>kineticlawObj</i> . For more information about creating <i>kineticlawObj</i> , see <code>sbioabstractkineticlaw</code> .
<i>unitObj</i>	Specify the user-defined unit to add to the library. For more information about creating <i>unitObj</i> , see <code>sbiounit</code> .
<i>unitprefixObj</i>	Specify the user-defined unit prefix to add to the library. For more information about creating <i>unitprefixObj</i> , see <code>sbiounitprefix</code> .

Description

The function `sbioaddtolibrary` adds kinetic law definitions, 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 kinetic law definition, unit, or unit prefix to the root object's `UserDefinedLibrary` property. These

library components become available automatically in future MATLAB sessions.

Use the kinetic law definitions 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')` and `(get(sbioroot, 'UserDefinedLibrary'))`.

To remove the library component from the user-defined library, use the function `sbioremovefromlibrary`. You cannot remove a kinetic law definition being used by a reaction.

Examples

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

- 1 Create a kinetic law definition.

```
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 kinetic law definition to the user-defined library.

```
sbioaddtolibrary(abstkineticlawObj);
```

The function adds the kinetic law definition 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 kinetic law definition when defining a reaction's kinetic law.

```
modelObj = sbiomodel('cell');  
reactionObj = addreaction(modelObj, 'A + B <-> B + C');  
kineticlawObj = addkineticlaw(reactionObj, 'ex_myLaw1');
```

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

See Also

`addkineticlaw`, `sbioabstractkineticlaw`, `sbioremovefromlibrary`,
`sbiroot`, `sbiunit`, `sbiunitprefix`

sbioconsmoiety

Purpose Find conserved moieties in SimBiology model

Syntax

```
[G, Sp] = sbioconsmoiety(mode1Obj)
[G, Sp] = sbioconsmoiety(mode1Obj, alg)
H = sbioconsmoiety(mode1Obj, alg, 'p')
H = sbioconsmoiety(mode1Obj, alg, 'p', FormatArg)
[SI, SD, LO, NR, ND] = sbioconsmoiety(mode1Obj, 'link')
```

Arguments

<i>G</i>	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 <i>G</i> specifies a linear combination of species whose rate of change over time is zero.
<i>Sp</i>	Cell array of species names that labels the columns of <i>G</i> . If the species are in multiple compartments, species names are qualified with the compartment name in the form <code>compartmentName.speciesName</code> . For example, <code>nucleus.DNA</code> , <code>cytoplasm.mRNA</code> .
<i>mode1Obj</i>	Model object to be evaluated for conserved moieties.
<i>alg</i>	Specify algorithm to use during evaluation of conserved moieties. Valid values are 'qr', 'rreduce', or 'semipos'.
<i>H</i>	Cell array of strings containing the conserved moieties.
<i>p</i>	Prints the output to a cell array of strings.
<i>FormatArg</i>	Specifies formatting for the output <i>H</i> . <i>FormatArg</i> should either be a C-style format string, or a positive integer specifying the maximum number of digits of precision used.
<i>SI</i>	Cell array containing the names of independent species in the model.

<i>SD</i>	Cell array containing the names of dependent species in the model.
<i>LO</i>	Link matrix relating SI and SD. The link matrix <i>LO</i> satisfies $ND = LO * NR$. For the 'link' functionality, species with their BoundaryCondition or ConstantAmount properties set to true are treated as having stoichiometry of zero in all reactions.
<i>NR</i>	Reduced stoichiometry matrices containing one row for each independent species. The concatenated matrix [<i>NR</i> ; <i>ND</i>] is a row-permuted version of the full stoichiometry matrix of <i>modelObj</i> .
<i>ND</i>	Reduced stoichiometry matrices containing one row for each dependent species. The concatenated matrix [<i>NR</i> ; <i>ND</i>] is a row-permuted version of the full stoichiometry matrix of <i>modelObj</i> .

Description

$[G, Sp] = \text{sbioconsmoiety}(\text{modelObj})$ 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.

$[G, Sp] = \text{sbioconsmoiety}(\text{modelObj}, \text{alg})$ 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, LO, NR, ND] = sbioconsmoiety(modelObj, 'link')` uses a QR-based algorithm to compute information relevant to the dimensional reduction, via conservation relations, of the reaction network in `modelObj`.

Examples

Example 1

This example shows conserved moieties in a cycle.

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

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

2 Look for conserved moieties.

```
[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_0pA + pol_0pB + pol_0pC'
     'OpB + pol_0pB + pA_0pB1 + pA_0pB_pA + pA_0pB2'
     'OpA + pol_0pA + pC_0pA1 + pC_0pA2 + pC_0pA_pC'
     'OpC + pol_0pC + pB_0pC1 + pB_0pC2 + pB_0pC_pB'
```

See Also

“Moiety Conservation” in the SimBiology User’s Guide documentation
 SimBiology method `getstoichmatrix`

sbioconvertunits

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, `sbioconvertunits` 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.

Examples 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:

```
modelObj = sbiomodel('cell');
compObj = addcompartment(modelObj, 'C');
speciesObj = addspecies (compObj, 'glucose', 23, 'InitialAmountUnits', 'molecule')
```

SimBiology Species Array

Index:	Compartment:	Name:	InitialAmount:	InitialAmountUnits:
1	C	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
```

The InitialAmount value is changed.

```
get (speciesObj, 'InitialAmount')
```

```
ans =
```

```
3.8192e-023
```

See Also

sbioshowunits

sbiocopylibrary

Purpose

Copy library to disk

Syntax

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

Description

`sbiocopylibrary` copies all user-defined kinetic law definitions to a file. `sbiocopylibrary ('kineticlaw', 'LibraryFileName')` copies all user-defined kinetic law definitions 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 kinetic law definitions that are in the built-in and user-defined libraries, use the commands `get(sbioroot, 'BuiltInKineticLaws')` and `get(sbioroot, 'UserDefinedKineticLaws')`. To add a kinetic law definition to the user-defined library, use the method `sbioaddtolibrary`.

To add a unit to the user-defined library, use the `sbioregisterunit` function. To add a unit prefix to the user-defined library, use the `sbioregisterunitprefix` function.

Examples

Create a kinetic law definition, add it to the user-defined library, and then copy the user-defined kinetic law library to a `.sbklib` file.

- 1 Create a kinetic law definition.

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

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

```
sbioaddtolibrary(abstkineticlawObj);
```

`sbioaddtolibrary` adds the kinetic law definition 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](#)

sbiodesktop

Purpose Open SimBiology modeling and simulation GUI

Syntax sbiodesktop
sbiodesktop(*mode1Obj*)

Arguments

<i>mode1Obj</i>	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 desktop, which lets you do the following:

- Build a SimBiology model by representing reaction pathways and entering 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 through individual or ensemble runs.
- View results from the simulation.
- Perform analysis tasks such as sensitivity analysis, parameter and species scans, and calculate conserved moieties.
- Create and/or modify user-defined units and unit prefixes.
- Create and/or modify user-defined kinetic laws.

sbiodesktop(*mode1Obj*) opens the SimBiology desktop with a top-level SimBiology model object (*mode1Obj*). If there is a project open in the SimBiology desktop, this command adds the model (*mode1Obj*) to the project. A top-level SimBiology model object has its property Parent set to the SimBiology root object. Thus, querying sbioroot at the command

line shows you all models in the MATLAB workspace, including the models available in the desktop. Any changes you make to the model at the command line are reflected in the desktop because both are pointing to the same model object in the `Root` object.

Note The `sbioreset` command removes all models from the root object and therefore this command also removes all models from the SimBiology desktop.

Examples

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

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

See Also

`sbioroot`, `simbiology`

sbiodose

Purpose Construct dose object

Syntax

```
doseObj = sbiodose('DoseName')
doseObj = sbiodose('DoseName', 'DoseType')
doseObj = sbiodose(...'PropertyName', PropertyValue...)
```

Inputs

<i>DoseName</i>	Name of the dose object.
<i>DoseType</i>	Selects which type of dose object to construct. Enter either 'schedule' or 'repeat'

- 'schedule' creates a ScheduleDose object and defines the dose with a time array, amount array, and rate array.
- 'repeat' creates a RepeatDose object and defines the dose with a dose amount, number of dose repetitions, and the time between doses.

Outputs

<i>doseObj</i>	ScheduleDose or RepeatDose object.
----------------	------------------------------------

Description

doseObj = sbiodose('DoseName') constructs a SimBiology RepeatDose object (*doseObj*), assigns *DoseName* to the property Name, and assigns [] to the property Parent.

doseObj = sbiodose('DoseName', 'DoseType') constructs either a SimBiology ScheduleDose object or RepeatDose object (*doseObj*).

doseObj = sbiodose(...'PropertyName', PropertyValue...) defines dose object properties. You can enter the property name/property value pairs 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 *doseObj* properties with the get command and modify *doseObj* properties with the set command.

Before you use a dose object in a simulation, you must add the object to a SimBiology model with the method `adddose`.

Examples

Construct a repeat dose object:

- 1 In the MATLAB Command Window, enter:

```
doseObj1 = sbiodose('dose1', 'repeat');
```

- 2 Define a repeating dose:

```
doseObj1.Amount      = 5;  
doseObj1.Repeat      = 6;  
doseObj1.Interval    = 24;  
doseObj1.TimeUnits   = 'hour';  
doseObj1.TargetName  = 'Central.x';
```

Construct a schedule dose object:

- 1 In the MATLAB Command Window, enter:

```
doseObj2 = sbiodose('dose2', 'schedule');
```

- 2 Define a dose schedule:

```
doseObj2.Time        = [0 24 48];  
doseObj2.Amount      = [10 5 5];  
doseObj2.TargetName  = 'Central.Drug';
```

See Also

Model object methods:

- `adddose` — add a dose object to a model object.
- `getdose` — get dose information from a model object.
- `removedose` — remove a dose object from a model object.

ScheduleDose object and RepeatDose object methods:

sbiodose

- `copyobj` — copy a dose object from one model object to another model object.
- `get` — view properties for a dose object.
- `set` — define or modify properties for a dose object.

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

<i>simdataObj</i>	An object that contains simulation data. You can generate a <i>simdataObj</i> object using the function <code>sbioenssemblerun</code> . All elements of <i>simdataObj</i> must contain data for the same states in the same model.
<i>Names</i>	Either a string or a cell array of strings. <i>Names</i> may include qualified names such as ' <i>CompartmentName.SpeciesName</i> ' or ' <i>ReactionName.ParameterName</i> ' to resolve ambiguities. Specifying {} for <i>Names</i> plots data for all states contained in <i>simdataObj</i> .
<i>Time</i>	A numeric scalar value. If the specified <i>Time</i> is not an element of the time vectors in <i>simdataObj</i> , then the function resamples <i>simdataObj</i> as necessary using linear interpolation.
<i>FH</i>	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 `sbioenssemblerun` 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

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

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

`sbioensemblerrun`, `sbioensemblestats`, `sbioemodel`

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

<i>simdataObj</i>	An object that contains simulation data generated by <code>sbioensemblerun</code> . All elements of <i>simdataObj</i> must contain data for the same states in the same model.
<i>modelObj</i>	Model object to be simulated.
<i>Numruns</i>	Integer scalar representing the number of stochastic runs to make.
<i>Interpolation</i>	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.

<i>configsetObj</i>	Specify the configuration set object to use in the ensemble simulation. For more information about configuration sets, see <code>Configset</code> object.
<i>variantObj</i>	Specify the variant object to apply to the model during the ensemble simulation. For more information about variant objects, see <code>Variant</code> 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 how to perform an ensemble run and generate a 2-D distribution plot.

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

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

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

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

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

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

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

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

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

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

See Also

`addconfigset`, `getconfigset`, `sbioensemblestats`,
`sbioensembleplot`, `setactiveconfigset`, `SimData` object

Purpose Get statistics from ensemble run data

Syntax

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

Arguments

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

<i>names</i>	Either a string or a cell array of strings. <i>names</i> may include qualified names such as ' <i>CompartmentName.SpeciesName</i> ' or ' <i>ReactionName.ParameterName</i> ' to resolve ambiguities. If you specify empty {} for <i>names</i> , <i>sbioensemblestats</i> returns statistics on all time courses contained in <i>simDataObj</i> .
<i>interpolation</i>	String variable denoting the interpolation method to be used if data is to be interpolated to get a consistent time vector. See <i>resample</i> 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 *sbioenssemblerun*.

`[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 = sbioensemblerrun(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

`sbioensemblerrun`, `sbioensembleplot`, `sbiogetnamedstate`, `sbiomodel`

sbioevent

Purpose Construct event object

Note sbioevent has been removed and produces an error. Use addevent instead.

Syntax

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

Arguments

<i>TriggerValue</i>	Required property to specify a trigger condition. Must be a MATLAB expression that evaluates to a logical value.
<i>EventFcnsValue</i>	A string or a cell array of strings, each of which specifies an assignment of the form ' <i>objectname</i> = <i>expression</i> ', where <i>objectname</i> is the name of a valid SimBiology object.
<i>PropertyName</i>	Property name for an event object from “Property Summary” on page 2-35.
<i>PropertyValue</i>	Property value. For more information on property values, see the property reference for each property listed in “Property Summary” on page 2-35.

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 “Changing Model Component Values Using Events” in the SimBiology User’s Guide documentation.

`eventObj = sbioevent(...'PropertyName', PropertyValue...)` defines optional properties. The property name/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

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

Property Summary

<code>Active</code>	Indicate object in use during simulation
<code>Annotation</code>	Store link to URL or file
<code>EventFcns</code>	Event expression
<code>Name</code>	Specify name of object
<code>Notes</code>	HTML text describing SimBiology object
<code>Parent</code>	Indicate parent object
<code>Tag</code>	Specify label for SimBiology object

sbioevent

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

addevent, copyobj, Event object

Purpose Plot status of sbionlmeFit

Syntax `stop = sbiofitstatusplot(beta, status, state)`

Description `stop = sbiofitstatusplot(beta, status, state)` initializes or updates a plot with the fixed effects, *beta*, the log likelihood *status.fval*, and the variance of the random effects, `diag(status.Psi)`.

The function returns an output (*stop*) to satisfy requirements for the 'OutputFcn' option of `nlmeFit`. For `sbiofitstatusplot`, the value of *stop* is always false.

Specify `sbiofitstatusplot` in the `sbiofit` function using the `optionstruc` (options structure) argument, to obtain status information about NLME fitting. Use `sbiofitstatusplot` or customize your own function to use in the options structure.

Inputs *beta*

The current fixed effects.

status

Structure containing several fields.

Field	Value
inner	Structure describing the current status of the inner iterations within the ALT and LAP procedures, with the fields: <ul style="list-style-type: none"> • procedure <ul style="list-style-type: none"> ▪ 'PNLS', 'LME', or 'none' when the procedure is 'ALT' ▪ 'PNLS', 'PLM', or 'none' when the procedure is 'LAP' • state — 'init', 'iter', 'done', or 'none'

Field	Value
	<ul style="list-style-type: none">iteration — Integer starting from 0, or NaN
procedure	'ALT' or 'LAP'
iteration	Integer starting from 0
fval	Current log-likelihood
Psi	Current random-effects covariance matrix
theta	Current parameterization of Psi
mse	Current error variance

state

Either 'init', 'iter', or 'done'.

Definitions

Alt

Alternating algorithm for the optimization of the LME or RELME approximations

FO

First-order estimate

FOCE

First-order conditional estimate

LAP

Optimization of the Laplacian approximation for FO or FOCE

LME

Linear mixed-effects estimation

NLME

Nonlinear mixed effects

PLM

Profiled likelihood maximization

PNLS

Penalized nonlinear least squares

RELME

Restricted likelihood for the linear mixed-effects model

Examples

Obtain status information for NLME fitting:

```
% Create options structure with 'OutputFcn'.
options.Options.OutputFcn = @sbiofitstatusplot;
% Pass options structure with OutputFcn to sbionlmeft function.
results = sbionlmeft(..., options);
```

See Also

[nlmeft](#) | [sbionlinfit](#) | [sbionlmeft](#)

How To

- “Obtaining the Status of Fitting”

sbiogetmodel

Purpose Get model object that generated simulation data

Syntax `modelObj = sbiogetmodel(simDataObj)`

Arguments

<code>simDataObj</code>	SimData object returned by the function <code>sbiosimulate</code> or by <code>sbioensemblrun</code> .
<code>modelObj</code>	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`

sbiogetnamedstate

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 an `n`-by-1 vector of time samples labeling the rows of `x`.
- `x` is an `n`-by-`m` matrix, where `n` is the number of times the reactions fired and `m` is the number of states logged during simulation. Each column of `x` defines the variation in the quantity of a species over time.

`[t,x] = sbiogetnamedstate(simDataObj,'Name')` returns the state data associated with the name `Name` from the `SimData` object (`smDataObj`), and returns it to `x`. `Name` can be a cell array names. If a name, `Name`, does not exist, you see a warning.

`[t,x,Name] = sbiogetnamedstate(...)` returns the names associated with each column of `x` to `Name`.

See Also `sbiosimulate`

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

<i>T</i>	Column vector of length <i>m</i> specifying time points for the sensitivity data in <i>R</i> .
<i>R</i>	An <i>m</i> -by- <i>n</i> -by- <i>p</i> array of sensitivity data with times, outputs, and input factors labeling its first, second, and third dimensions respectively.
<i>Outputs</i>	Contains names of the species states that label the second dimension of <i>R</i> . $R(:, i, j)$ is the time course for the sensitivity of state <i>Outputs</i> { <i>i</i> } to the input factor <i>Inpfacs</i> { <i>j</i> }. When <i>simdataObj</i> contains more than one element, the output arguments are cell arrays in which each cell contains data for the corresponding element of <i>simdataObj</i> .
<i>Inpfacs</i>	Contains names of the input factors that label the third dimension of <i>R</i> . $R(:, i, j)$ is the time course for the sensitivity of states <i>Outputs</i> { <i>i</i> } to the input factor <i>Inpfacs</i> { <i>j</i> }.
<i>simDataObj</i>	SimData object returned by <code>sbiosimulate</code> . Contains sensitivity data when sensitivity analysis is enabled.

sbiogetsensmatrix

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

Description

`[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`

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`.

You can get general information on the SimBiology software by specifying *FunctionName* as 'sbio'. General information about a SimBiology object can be returned by specifying *FunctionName* as one of the following:
'AbstractKineticLaw', 'Compartment', 'CompileOptions',
'Configset', 'Event', 'ExplicitTauSolverOptions',
'ImplicitTauSolverOptions', 'KineticLaw', 'ODESolverOptions',
'Model', 'Parameter', 'PKData', 'PKCompartment', 'PKModelDeign',
'PKModelMap', 'Reaction', 'Root', 'Rule', 'RuntimeOptions',
'SensitivityAnalysisOptions', 'SimData', 'Species',
'SSASolverOptions', 'Library', 'Unit', 'UnitPrefix', or
'Variant'.

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

See Also MATLAB function help

sbiolasterror

Purpose SimBiology last error message

Syntax
sbiolasterror
diagstruct = sbiolasterror
sbiolasterror([])
sbiolasterror(*diagstruct*)

Arguments

<i>diagstruct</i>	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 the software. The fields of the diagnostic structure are:

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

sbiolastwarning

Purpose SimBiology last warning message

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

Arguments

<i>diagstruct</i>	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 the software. The fields of the diagnostic structure are:

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

`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`

Purpose

Load project from file

Syntax

```
sbioloadproject('projFilename')  
sbioloadproject ('projFilename','variableName')  
sbioloadproject projFilename variableName1 variableName2...  
s = sbioloadproject (...)
```

Description

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

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

`sbioloadproject projFilename variableName1 variableName2...` loads the specified variables from the project.

`s = sbioloadproject (...)` returns the contents of *projFilename* in a variable `s`. `s` is a struct containing fields matching the variables retrieved from the SimBiology project.

You can display the contents of the project file using the `sbiowhos` command.

See Also

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

Purpose Construct model object

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

Arguments

<i>NameValue</i>	Required property to specify a unique name for a model object. Enter a character string.
<i>PropertyName</i>	Property name for a Model object from “Property Summary” on page 2-54.
<i>PropertyValue</i>	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/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

<code>addcompartment (model, compartment)</code>	Create compartment object
<code>addconfigset (model)</code>	Create configuration set object and add to model object

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

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

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 a 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, copyobj, get, sbioroot, sbiosimulate, set

Purpose

Nonlinear least-squares regression using SimBiology models

Syntax

```
results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj,
    Beta0)
results = sbionlmeft(modelObj, pkModelMapObject,
    pkDataObject, Beta0, 'ParameterName',ParameterValue)
results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj,
    Beta0, ...)
[results, SimDataI] = sbionlinfit(...)
```

Description

Note This function requires `nlinfit` in Statistics Toolbox™ (Version 7.0 or later).

`results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, Beta0)` performs least-squares regression using the SimBiology model, `modelObj` and returns estimated results in the `results` structure.

`results = sbionlmeft(modelObj, pkModelMapObject, pkDataObject, Beta0, 'ParameterName',ParameterValue)` accepts one or more comma-separated parameter name/value pairs that are accepted by `nlinfit`. In addition, lets you specify a transformation function for each of the estimated parameters using `ParamTransform`.

`results = sbionlinfit(modelObj, pkModelMapObject, pkDataObj, Beta0, ...)` lets you supply additional arguments accepted by `nlinfit`. See `nlinfit` in the Statistics Toolbox User's Guide for information on the accepted properties.

`[results, SimDataI] = sbionlinfit(...)` returns simulations of the SimBiology model, `modelObj`, using the estimated values of the parameters.

Input Arguments

`modelObj`

SimBiology model object used to fit observed data.

`pkModelMapObject`

PKModelMap object that defines the roles of the model components in the estimation. For more information, see PKModelMap object.

pkDataObj

PKData object that defines the data to use in fitting, and the roles of the data columns used for estimation. For more information, see PKData object.

Beta0

A vector of initial estimates for the fixed effects. The length of *Beta0* must equal at least the length of *modelMapObject.Estimated*. The final estimates for the fixed effects defined in *Beta0* are log transformed in the results.

For more information on specifying initial estimates, see “Setting Initial Estimates” in the SimBiology documentation.

Parameter Name/Value Pairs

This section contains a partial list of supported name/value pairs. For a complete list, see *nlinfit* in the Statistics Toolbox documentation.

ParamTransform

A vector of values specifying a transformation function $f()$ for each of the estimated parameters: $\text{estimate} = f(\text{Beta})$. Each element of the vector must be one of the following integer codes specifying the transformation for the corresponding value of estimate:

- 0 – $\text{estimate} = \text{Beta}$
- 1 – $\log(\text{estimate}) = \text{Beta}$ (default for all parameters).
- 2 – $\text{probit}(\text{estimate}) = \text{beta}$
- 3 – $\text{logit}(\text{estimate}) = \text{beta}$

For more information, see “Specifying Parameter Transformations” in the SimBiology documentation.

Output Arguments

results

A structure with the following fields:

- *estimate* — Fitted coefficients
- *beta* — Fitted coefficients in transformed space
- *R* — Residuals
- *J* — Jacobian of the model
- *COVB* — Estimated covariance matrix for the fitted coefficients
- *mse* — Estimate of the error of the variance term

SimDataI

SimDataI contains simulation results for individuals.

See Also

PKData object | PKModelDesign object | PKModelDesign object | PKModelMap object | Model object | sbionlmeft | nlinfit

Purpose

Estimate nonlinear mixed effects using SimBiology models

Syntax

```
results = sbionlmeft(modelObj, pkModelMapObject,
    pkDataObject, Beta0)
results = sbionlmeft(modelObj, pkModelMapObject,
    pkDataObject, Beta0, 'ParameterName',ParameterValue)
... = sbionlmeft(..., optionStruct)
[results, SimDataI, SimDataP] = sbionlmeft(...)
```

Description

Note This function requires nlmefit in Statistics Toolbox (Version 7.0 or later).

`results = sbionlmeft(modelObj, pkModelMapObject, pkDataObject, Beta0)` performs nonlinear mixed effects estimation using the SimBiology model, `modelObj` and returns estimated results in the `results` structure.

`results = sbionlmeft(modelObj, pkModelMapObject, pkDataObject, Beta0, 'ParameterName',ParameterValue)` accepts one or more comma-separated parameter name/value pairs that are accepted by `nlmefit`. Specify `ParameterName` inside single quotes.

`... = sbionlmeft(..., optionStruct)` where `optionStruct` lets you construct a `struct` that contains field names that are the parameter names accepted by `nlmefit` and field values that are the associated parameter values.

SimBiology software contains a function (`sbiofitstatusplot`) that you can specify in the options structure. This function lets you monitor the status of fitting.

`[results, SimDataI, SimDataP] = sbionlmeft(...)` returns simulation data of the SimBiology model, `modelObj`, using the estimated values of the parameters.

Input Arguments

modelObject

SimBiology model object used to fit observed data.

pkModelMapObject

PKModelMap object that defines the roles of the model components used for estimation. For more information, see PKModelMap object.

pkDataObject

PKData object that defines the data to use in fitting and the roles of the columns used for estimation. *pkDataObject* must define target data for at least two groups. For more information, see PKData object.

Beta0

A vector of initial estimates for the fixed effects. The first P elements of *Beta0* correspond to the fixed effects for each of the P elements of *modelMapObject.Estimated*. Additional elements correspond to the fixed effects for covariate factors. The first P elements of *Beta0* are transformed as specified by the ParamTransform nlmeffit option (log transformed by default). For more information on specifying initial estimates see in the SimBiology documentation.

optionStruct

A struct that can contain fields and values where the field names are the parameter-names accepted by nlmeffit and the field values are the associated parameter-values.

Parameter Name/Value Pairs

This section contains a partial list of supported name/value pairs. For a complete list, see nlmeffit in the Statistics Toolbox documentation.

FEGroupDesign

Specify the design matrix for each of the groups. See “Specifying the Covariate Model” in the SimBiology documentation.

ParamTransform

Specify how the parameters are distributed. The available distributions are: `none`, `log`, `probit`, and `logit`. See “Specifying Parameter Transformations” in the SimBiology documentation.

Default: `log`

See `nlmefit` in the Statistics Toolbox documentation for information on all the accepted properties including `FEGroupDesign`, and `ParamTransform`.

The following parameter name/value pairs are not supported:

- `FEConstDesign`
- `FEObsDesign`
- `FEParamsSelect`
- `REConstDesign`
- `REGroupDesign`
- `REObsDesign`
- `Vectorization`
- `Jacobian`

Output Arguments

results

A structure with the following fields:

- A `results` structure containing
 - `estimate` — Estimates for the fixed effects.
 - `phiP` — Estimated parameter values for the population
 - `phiI` — Estimated parameter values for individuals
 - `beta` — Estimates for the fixed effects in transformed space as specified in the `ParamTransform` option.

sbionlmeffit

- `psi` — Estimated covariance matrix of the random effects
- `stats` — Structure with statistics such as AIC, and BIC. For a complete list see `nlmefit` in the Statistics Toolbox documentation.
- `b` — Estimated random effects for each group in *observedData*

SimDataI

SimDataI contains the data from simulating the model using the estimated parameter values, for individuals.

SimDataP

SimDataP contains the data from simulating the model using the estimated parameter values, for the population.

See Also

PKData object | PKModelDesign object | PKModelMap object | Model object | sbiofitstatusplot | sbionlinfit | sbionlmeffitsa | nlmefit

How To

- “Fitting Pharmacokinetic Model Parameters at the Command Line”

Purpose

Estimate nonlinear mixed effects with stochastic EM algorithm

Syntax

```

results = sbionlmefitsa(modelObj, pkModelMapObject,
    pkDataObject, Beta0)
results = sbionlmefitsa(modelObj, pkModelMapObject,
    pkDataObject, Beta0, 'ParameterName',ParameterValue)
... = sbionlmefitsa(..., optionStruct)
[results, SimDataI, SimDataP] = sbionlmefitsa(...)

```

Description

Note This function requires nlmefitsa in Statistics Toolbox (Version 7.0 or later).

results = sbionlmefitsa(*modelObj*, *pkModelMapObject*, *pkDataObject*, *Beta0*) estimations using the Stochastic Approximation Expectation-Maximization (SAEM) algorithm for fitting population data with the SimBiology model, *modelObj* and returns the estimated results in the *results* structure.

results = sbionlmefitsa(*modelObj*, *pkModelMapObject*, *pkDataObject*, *Beta0*, 'ParameterName',*ParameterValue*) accepts one or more comma-separated parameter name/value pairs that are accepted by nlmefitsa. Specify *ParameterName* inside single quotes.

... = sbionlmefitsa(*...*, *optionStruct*) lets you construct a struct that contains field names that are the parameter names accepted by nlmefitsa and field values that are the associated parameter values.

SimBiology software contains a function (sbiofitstatusplot) that you can specify in the options structure. This function lets you monitor the status of fitting.

[*results*, *SimDataI*, *SimDataP*] = sbionlmefitsa(*...*) returns simulation data of the SimBiology model, *modelObj*, using the estimated values of the parameters.

Input Arguments

modelObject

SimBiology model object used to fit observed data.

pkModelMapObject

PKModelMap object that defines the roles of the model components used for estimation. For more information, see PKModelMap object.

pkDataObject

PKData object that defines the data to use in fitting and the roles of the columns used for estimation. *pkDataObject* must define target data for at least two groups. For more information, see PKData object.

Beta0

A vector of initial estimates for the fixed effects. The first P elements of *Beta0* correspond to the fixed effects for each of the P elements of *modelMapObject.Estimated*. Additional elements correspond to the fixed effects for covariate factors. The first P elements of *Beta0* are transformed as specified by the ParamTransform *nlmefit* option (log transformed by default). For more information on specifying initial estimates see in the SimBiology documentation.

optionStruct

A struct that can contain fields and values where the field names are the parameter names accepted by *nlmefitsa* and the field values are the associated parameter values.

Parameter Name/Value Pairs

This section contains a partial list of supported name/value pairs. For a complete list, see *nlmefitsa* in the Statistics Toolbox documentation.

ErrorModel

Specify the error term. The available error models are:

- constant
- proportional
- combined
- exponential

See “Specifying an Error Model” in the SimBiology documentation.

Default: constant

FEGroupDesign

Specify the design matrix for each of the groups. See in the SimBiology documentation.

ParamTransform

Specify parameter transformations. The available transformations are: none, log, probit, and logit. See “Specifying Parameter Transformations” in the SimBiology documentation.

Default: log

See `nlmefitsa` in the Statistics Toolbox documentation for information on all the accepted properties including `FEGroupDesign`, `ParamTransform` and `ErrorModel`.

The following parameter name/value pairs are not supported:

- FEConstDesign
- FEObsDesign
- FEParamsSelect
- REConstDesign
- REGroupDesign
- REObsDesign

- Vectorization
- Jacobian

Output Arguments

results

A structure with the following fields:

- A *results* structure containing
 - *estimate* — Estimates for the fixed effects.
 - *phiP* — Estimated parameter values for the population
 - *phiI* — Estimated parameter values for individuals
 - *beta* — Estimates for the fixed effects in transformed space as specified in the *ParamTransform* option.
 - *psi* — Estimated covariance matrix of the random effects
 - *stats* — Structure with statistics such as AIC, and BIC. For a complete list see *nlmefitsa* in the Statistics Toolbox documentation.
 - *b* — Estimated random effects for each group in *observedData*

SimDataI

SimDataI contains the data from simulating the model using the estimated parameter values, for individuals.

SimDataP

SimDataP contains the data from simulating the model using the estimated parameter values, for the population.

See Also

PKData object | PKModelDesign object | PKModelMap object | Model object | sbiofitstatusplot | sbionlinfit | sbionlmefit | nlmefit

How To

.

sbionmfiledef

Purpose NONMEM file definition object for sbionmimport

Syntax
`nmdefObj = sbionmfiledef`
`nmdefObj = sbionmfiledef('PropertyName', PropertyValue)`

Description `nmdefObj = sbionmfiledef` creates a NONMEM file definition object. The NONMEM file definition object contains properties for specifying the NONMEM data items such as group, time, and dependent variable. The NONMEM file definition object lets you configure the properties to the column heading or the index of the column. Use the NONMEM file definition object in conjunction with the `sbionmimport` function to import NONMEM formatted files for use in fitting.

`nmdefObj = sbionmfiledef('PropertyName', PropertyValue)` accepts one or more comma-separated property name/value pairs. Specify *PropertyName* inside single quotes. To see the default interpretations for NONMEM formatted files see “Support for Importing NONMEM Formatted Files” in the SimBiology documentation.

- Tips**
- Use `sbionmfiledef` with `sbionmimport` if you want to apply NONMEM interpretation of headers, and the data file has column header labels different from the table shown in “Support for Importing NONMEM Formatted Files”
 - Use `sbionmimport` if the data file has column header labels identical to the table shown in “Support for Importing NONMEM Formatted Files”.

Input Arguments

Filename

If *Filename* extension is `.xls` or `.xlsx` it is assumed to be an Excel® file, otherwise it is assumed to be a text file. `sbionmfiledef` file reads the file using the dataset constructor.

Property Name/Value Pairs

CompartmentLabel

Identifies the column in the NONMEM formatted file that contains the compartment. Specify the header name as a char string or specify the index number of the header. During import the `sbionmimport` function uses the information in the column to interpret which compartment receives a dose or measured an observation. The `EventIDLabel` property specifies whether the value is a dose or an observation.

Default: ''

ContinuousCovariateLabels

Identifies the column in the NONMEM formatted file that contains continuous covariates. Specify the header name as a char string or specify the index number of the header.

Default: {}

DateLabel

Identifies the column in the NONMEM formatted file that contains the date. Specify the header name as a char string or specify the index number of the header. During import the `sbionmimport` function uses the information in the column to interpret time information for each dose, response and covariate measurements.

Default: ''

DependentVariableLabel

Identifies the column in the NONMEM formatted file that contains observations. Specify the header name as a char string or specify the index number of the header. During import the `sbionmimport` function uses the information in the column to interpret date and time information for each dose and response.

Default: ''

DoseLabel

Identifies the column in the NONMEM formatted file that contains the dosing information. Specify the header name as a char string or specify the index number of the header.

Default: ''

DoseIntervallLabel

Identifies the column in the NONMEM formatted file that contains the time between doses. Specify the header name as a char string or specify the index number of the header.

Default: ''

DoseRepeatLabel

Identifies the column in the NONMEM formatted file that contains the number of times (excluding the initial dose) that the dose is repeated. Specify the header name as a char string or specify the index number of the header.

Default: ''

EventIDLabel

Identifies the column in the NONMEM formatted file that contains the event identification specifying whether the value is a dose, observation, or covariate. Specify the header name as a char string or specify the index number of the header.

Default: ''

GroupLabel

Identifies the column in the NONMEM formatted file that contains the Group ID. Specify the header name as a char string or specify the index number of the header.

Default: ''

MissingDependentVariableLabel

Identifies the column in the NONMEM formatted file that contains information about whether a row contains an observation event (0), or not (1). Specify the header name as a char string or specify the index number of the header.

Default: ''

RateLabel

Identifies the column in the NONMEM formatted file that contains the rate of infusion. Specify the header name as a char string or specify the index number of the header.

Default: ''

TimeLabel

Identifies the column in the NONMEM formatted file that contains the time or date of observation. During import the `sbionmimport` function uses this information to interpret when a dose was given, an observation or covariate measurement recorded. Specify the header name as a char string or specify the index number of the header.

Default: ''

Type

Identifies the object as 'NMFileDef', (Read-only).

Output Arguments

nmdefObj

Defines the meanings of the file column headings. It contains properties for specifying data items such as group, time and date. TimeLabel and DependentVariableLabel must be specified.

sbionmfiledef

Examples

Configure a NONMEM file definition object and import data from a NONMEM formatted file.

```
% Configure a NMFileDef object.
def = sbionmfiledef;
def.CompartmentLabel      = 'CPT';
def.DoseLabel             = 'AMT';
def.DoseIntervalLabel    = 'II';
def.DoseRepeatLabel       = 'ADDL';
def.GroupLabel            = 'ID';
def.TimeLabel             = 'TIME';
def.DependentVariableLabel = 'DV';
def.EventIDLabel          = 'EVID';

filename = 'C:\work\datafiles\dose.xls';
ds = sbionmimport(filename, def);
```

See Also

sbionmimport

How To

- “Importing Data at the Command Line”
- “Importing Data into the SimBiology Desktop”

Purpose

Import NONMEM formatted data

Syntax

```

simbioDataset = sbionmimport('Filename')
simbioDataset = sbionmimport (nmds)
simbioDataset = sbionmimport('Filename', nmdefObj)
simbioDataset = sbionmimport('Filename', nmdefObj,
    'ParameterName', ParameterValue)
simbioDataset = sbionmimport(nmds, nmdefObj)
[simbioDataset, PKDataObj] = sbionmimport(...)

```

Description

`simbioDataset = sbionmimport('Filename')` or `simbioDataset = sbionmimport (nmds)` converts a NONMEM formatted file, and assumes that the file is configured to use the following default values for column headers: ADDL, AMT, CPT, DATE, DAT1, DAT2, or DAT3, DV, EVID, ID, II, MDV, RATE, TIME. See “Support for Importing NONMEM Formatted Files” in the SimBiology documentation for more information on each of the headers.

`simbioDataset = sbionmimport('Filename', nmdefObj)` imports a NONMEM formatted file named *Filename*, into a SimBiology formatted data set, *simbioDataset*, using the meanings of the file column headings defined in the NONMEM file definition object (*nmdefObj*).

`simbioDataset = sbionmimport('Filename', nmdefObj, 'ParameterName', ParameterValue)` accepts one or more comma-separated parameter name/value pairs that are accepted by the `dataset` function. If `dataset` requires additional information to read the file such as the delimiter, specify these as property value pairs in `sbionmimport`. See `dataset` in the Statistics Toolbox documentation for a list of supported property value pairs.

`simbioDataset = sbionmimport(nmds, nmdefObj)` converts a NONMEM formatted dataset array (*nmds*), into a SimBiology formatted data set.

`[simbioDataset, PKDataObj] = sbionmimport(...)` returns a PKData object, *PKDataObj* containing the data set *simbioDataset*. The *PKDataObj* properties show the labels specified in *simbioDataset*.

sbionmimport

Input Arguments

Filename

If extension of *Filename* is .xls or .xlsx, sbionmimport assumes it to be an Excel file. Otherwise sbionmimport assumes *Filename* is a text file. sbionmimport reads the file using the dataset constructor.

nmds

nmds is a NONMEM formatted dataset object, in other words a NONMEM formatted file imported using the dataset command. For more information see dataset in the Statistics Toolbox documentation.

nmdefObj

nmdefObj defines the meanings of the file column headings. *nmdefObj* is a NONMEM file definition object created using the sbionmfiledef function. It contains properties for specifying data items such as group, time, and date. You must specify the TimeLabel and the DependentVariableLabel properties.

Output Arguments

simbioDataset

The SimBiology formatted data set uses a separate column for each dose and observation. The Description property of *simbioDataset* contains a list of warnings that occurred while constructing *simbioDataset*. To view the warnings enter: get(*simbioDataset*, 'Description').

PKDataObj

The PKData object defines the data to use in fitting and the roles of the columns used for estimation. For more information, see PKData object.

See Also

sbionmfiledef

How To

- “Importing Data at the Command Line”

- “Importing Data into the SimBiology Desktop”

sbioparamestim

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

<i>k</i>	Vector of estimated parameter values. For all optimization methods except 'fminsearch' the parameters are constrained to be greater than or equal to zero.
<i>result</i>	struct with fields that provide information about the progress of optimization.
<i>tspan</i>	An n-by-1 vector representing the time span of the target data <i>xtarget</i> .
<i>xtarget</i>	An n-by-m matrix, where n is the number of time samples and m is the number of states you would like to match during the simulation. States can only be species varying with time. You cannot use time varying (nonconstant) parameters. The number of rows of <i>xtarget</i> must be the same as the number of rows of <i>tspan</i> .

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

<i>k0</i>	Array of doubles that holds initial values of parameters to be estimated. The length of <i>k0</i> is same as that of <i>parameter_array</i> . When you specify <i>k0</i> , <i>sbioparamestim</i> ignores any initial values specified in active variants attached to the model. If left unspecified, <i>sbioparamestim</i> takes initial values for parameters from the model (<i>modelObj</i>) or, if there are active variants, <i>sbioparamestim</i> uses any initial values specified in the active variants. See <code>Variant</code> object for more information about variants.
<i>method</i>	<p>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'.</p> <p>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 <code>optimset</code>, <code>gaoptimset</code>, or <code>psoptimset</code>.</p> <p><i>sbioparamestim</i> uses the cell array option to specify user-defined optimization options.</p> <p>Note that 'fminsearch' is an unconstrained optimization method and this could result in negative values for parameters.</p>

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. If the Optimization Toolbox™ product is installed, `sbioparamestim` uses `lsqnonlin` for parameter estimation. If the Optimization Toolbox product is not installed, `sbioparamestim` uses `fminsearch`.

`[...]= sbioparamestim(..., species_array, parameter_array, k0)` lets you specify the initial values of parameters.

`[...]= sbioparamestim(..., species_array, parameter_array, k0, method)` lets you specify the optimization method to use.

Examples

Example 1

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

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

```
sbioloadproject gprotein_norules m1;
```

- 2 Store the target data in a variable.

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

- 3 Store all model parameters in an array.

```
p_array = sbioselect(m1, 'Type', 'parameter');
```

- 4 Store the species that should match target.

```
Ga = sbioselect(m1, 'Type', 'species', 'Name', 'Ga');
% In this example only one species is selected.
```

sbioparamestim

```
% To match more than one targeted species data
% replace with selected species array.
```

5 Estimate the parameters.

```
[k, result] = sbioparamestim(m1, tspan, xtarget, Ga, p_array)
```

```
k =
```

```
0.1988
0.0000
0.0045
6.2859
0.0040
0.9726
0.0000
0.1164
```

```
result =
```

```
    fval: 8.7248e+005
  residual: [9x1 double]
  exitflag: 2
 iterations: 2
  funccount: 27
 algorithm: 'large-scale: trust-region reflective Newton'
  message: [1x77 char]
```

Example 2

Estimate parameters specified in `p_array` and species specified in `sp_array` using different algorithms. This example uses the data from “Example 1” on page 2-79.

```
[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 2-79.

```
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`

Global Optimization Toolbox functions `gaoptimset`, `psoptimset`

sbioparameter

Purpose Construct parameter object

Note sbioparameter has been removed and produces an error. Use addparameter instead.

Syntax

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

Arguments

<i>Obj</i>	Model object or kinetic law object.
<i>NameValue</i>	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.
<i>ValueValue</i>	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 (parameterObj) 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

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

sbioparameter

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

<i>simDataObj</i>	SimBiology data object.
<i>fcnHandleValue</i>	Function handle.
<i>xArgsValue</i>	Cell array with the names of the states.
<i>yArgsValue</i>	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 the SimBiology data object, *simDataObj*, in the same figure. The plot is created by calling the function handle, *fcnHandleValue*, with input arguments *simDataObj*, *xArgsValue*, and *yArgsValue*.

xArgsValue and *yArgsValue* should be cell arrays with the names of the states. The function represented by the function handle should return an array of handles and names. The signature of the function is shown below.

```
function [handles, names] = functionName(simDataObj, xArgsValue, YArgsValue)
```

The output argument `handles` is a two-dimensional array of handles to the lines plotted by the function. Each column corresponds to a run and each row corresponds to the lines being plotted for a state. `names` is a one-dimensional cell array that contains the names to be displayed on the nodes which are children of a Run Node. The length of `names` should be equal to the number of rows in the `handles` array returned.

Examples

This example shows how to plot data from an ensemble run without interpolation.

```
% Load the radiodecay model.
sbioloadproject('radiodecay.sbproj','m1');

% Configure the model to run with the stochastic solver.
cs = getconfigset(m1, 'active');
set(cs, 'SolverType', 'ssa');
set(cs.SolverOptions, 'LogDecimation', 100);

% Run an ensemble simulation and view the results.
simDataObj = sbioenssemblerun(m1, 10, 'linear');
sbioplot(simDataObj);
```

See Also

`sbiosubplot`

sbioreaction

Purpose

Construct reaction object

Note sbioreaction has been removed and produces an error. Use addreaction instead.

Syntax

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

Arguments

<i>ReactionValue</i>	Specify the reaction equation. Enter a character string. A hyphen preceded by a space and followed by a right angle bracket (->) indicates reactants going forward to products. A hyphen with left and right angle brackets (<->) indicates a reversible reaction. Coefficients before reactant or product names must be followed by a space. Examples are 'A -> B', 'A + B -> C', '2 A + B -> 2 C', 'A <-> B'.
<i>ReactantsValue</i>	A string defining the species name, a cell array of strings, a species object or an array of species objects.
<i>ProductsValue</i>	A string defining the species name, a cell array of strings, a species object or an array of species objects.

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

Method Summary

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

Property Summary

Active	Indicate object in use during simulation
Annotation	Store link to URL or file
KineticLaw	Show kinetic law used for ReactionRate
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Products	Array of reaction products
Reactants	Array of reaction reactants
Reaction	Reaction object reaction
ReactionRate	Reaction rate equation in reaction object
Reversible	Specify whether reaction is reversible or irreversible
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 = sbireaction('a + 3 b -> 2 c');
reactionObj2 = sbireaction({'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

`addrreaction`, `sbiomodel`

Purpose Create user-defined unit

Note `sbioregisterunit` has been removed and produces an error. Use `sbiounit` followed by `sbioaddtolibrary` instead.

Syntax

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

Description

`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 used 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.

sbioregisterunit

See Also

`sbioaddtolibrary`, `sbioremovefromlibrary`, `sbioshowunits`,
`sbiounit`

Purpose Create user-defined unit prefix

Note `sbioregisterunitprefix` has been removed and produces an error. 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 kinetic law, unit, or unit prefix from library

Syntax
`sbioremovefromlibrary (Obj)`
`sbioremovefromlibrary ('Type', 'Name')`

Description `sbioremovefromlibrary (Obj)` removes the kinetic law definition, 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 a kinetic law definition that is being used in a model.

You can use a built-in or user-defined kinetic law definition when you construct a kinetic law object with the method `addkineticlaw`.

`sbioremovefromlibrary ('Type', 'Name')` removes the object of type 'Type' with name 'Name' from the corresponding user-defined library. Type can be 'kineticlaw', 'unit' or 'unitprefix'.

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

To create a kinetic law definition, unit, or unit prefix, use `sbioabstractkineticlaw`, `sbiounit`, or `sbiounitprefix` respectively.

To add a kinetic law definition, unit, or unit prefix to the user-defined library, use the function `sbioaddtolibrary`.

Example

This example shows how to remove a kinetic law definition from the user-defined library.

- 1 Create a kinetic law definition.

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

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

```
sbioaddtolibrary(abstkineticlawObj);
```


`sbioaddtolibrary` adds the kinetic law definition 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 kinetic law definition.

```
sbioremovefromlibrary('kineticlaw', 'mylaw1');
```

See Also

`sbioaddtolibrary`, `sbioabstractkineticlaw`, `sbiounit`,
`sbiounitprefix`

sbioreset

Purpose Delete all model and simulation objects

Syntax `sbioreset`

Description `sbioreset` deletes all SimBiology model and simulation objects at the root level. You cannot use a SimBiology model or simulation object after it is deleted. You should remove objects from the MATLAB workspace with the function `clear`. If the SimBiology desktop is open, note that calling `sbioreset` at the command line also deletes model and data objects that are open in the desktop.

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 a kinetic law definition 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.

Note

Example

This example shows 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** Use `clear all` to clear the workspace. 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** Use `sbioreset` to delete the `modelObj` from the root.

```
sbioreset
rootObj
```

```
SimBiology Root Contains:
```

```

Models:                            0
Builtin Abstract Kinetic Laws:      3
User Abstract Kinetic Laws:         0
Builtin Units:                      54

```

sbioreset

User Units:	0
Builtin Unit Prefixes:	13
User Unit Prefixes:	0

See Also

sbioroot

Purpose Return SimBiology root object

Syntax `rootObj = sbioroot`

Arguments

<code>rootObj</code>	Return sbioroot to this 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 kinetic laws.

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 kinetic laws define the built-in kinetic laws and user-defined kinetic laws. See `AbstractKineticLaw` object for more information.

To add a unit, prefix or kinetic law to the root (in the user-defined library), use the `sbioaddtolibrary` function. To remove, use `sbioremovefromlibrary`.

The models opened in the SimBiology desktop are stored in the root object.

Method Summary

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

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

`addkineticlaw`, `sbiomodel`, `sbioreset`

Purpose Construct rule object

Note sbiorule has been removed and produces an error. Use addrule instead.

Syntax

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

Arguments

RuleValue Enter a character string within quotation marks. For example, enter the algebraic rule 'Va*Ea + Vi*Ei - K2'.

RuleTypeValue Enter 'algebraic', 'initialassignment', 'repeatedAssignment', or 'rate'. See RuleType for more information.

Description

A SimBiology rule is a mathematical expression that modifies a species amount, or a parameter value. A rule is a MATLAB expression that uses species, and parameters.

`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

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

Property Summary

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

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

Examples

Example 1

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

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

Example 2

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

```
help(ruleObj, 'RuleType')
```

Example 3

List the properties for a rule.

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

See Also

addrule, copyobj, sbiomodel

sbiosaveproject

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 `sbioimportproject`. `sbiosaveproject` returns an error if `projFilename.sbproj` is not writable.

`sbiosaveproject` creates the binary SimBiology project file named `simbiology.sbproj`. `sbiosaveproject` 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 (projFileName, '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

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

sbioselect

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

Arguments

<i>Out</i>	Object or array of objects returned by the <code>sbioselect</code> function. <i>Out</i> might contain a mixture of object types (for example, species and parameters), depending on the selection you specify. If <i>PropertyValue</i> is a cell array, then the function returns all objects with the property ' <i>PropertyName</i> ' that matches any element of <i>PropertyValue</i> .
<i>Obj</i>	SimBiology object or array of objects to search. If an object is not specified, <code>sbioselect</code> searches the root.
<i>PropertyName</i>	Any property of the object being searched.
<i>PropertyValue</i>	Specify <i>PropertyValue</i> to include in the selection criteria.
<i>TypeValue</i>	Type of object to include in the selection, for example, <code>sbioModel</code> , <code>species</code> , <code>reaction</code> , or <code>kineticLaw</code> .
<i>Condition</i>	The search condition. See the table under “Description” on page 2-109 for a list of conditions.

<i>PropertyNameCondition</i>	Search condition that applies only to property names (which are strings). See the table listing “Conditions for Properties Names or String Values” below.
<i>PropertyNamePattern</i>	String used to select the property name according to the condition imposed by <i>PropertyNameCondition</i> .
<i>DepthValue</i>	Specify the depth number to search. Valid numbers are positive integer values and <i>inf</i> . If <i>DepthValue</i> is <i>inf</i> , <i>sbioselect</i> searches <i>Obj</i> and all of its children. If <i>DepthValue</i> is 1, <i>sbioselect</i> only searches <i>Obj</i> and not its children. By default, <i>DepthValue</i> is <i>inf</i> .

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*). If the property name in a property-value pair contains either a '?' or '*', then the name is automatically interpreted as a wildcard expression, equivalent to the where clause (*'Where', 'wildcard', 'PropertyName', '==', PropertyValue*).

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 match 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.

`Out = sbioselect(Obj, 'Where', 'PropertyNameCondition', 'PropertyNamePattern', 'Condition', PropertyValue)` finds objects with a property name that matches the pattern in (*PropertyNamePattern*) with the condition (*PropertyNameCondition*) and matches the value (*PropertyValue*) with the condition (*Condition*). Use this syntax when you want search conditions on both property names and property values.

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

sbioselect

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

Conditions for Numeric Properties	Example Syntax
<p>equal_and_same_type</p>	<p>Similar to ==, but in addition requires the property value to be of the same type. Search in the model object (modelObj), and return all objects containing a property of type double and a value equal to 0. (Using '==' would also select objects containing a property with a value of false.)</p> <pre> zeroObj = sbioselect(modelObj, ... 'Where', '*', 'equal_and_same_type', 0); </pre>
<p>unequal_and_same_type</p>	<p>Similar to ~=, but in addition requires the property value to be of the same type. Select all objects containing a property of type double and value not equal to 0. (Using '~=' would also select objects containing a property with a value of true.)</p> <pre> nonzeroObj = sbioselect(modelObj, ... 'Where', '*', 'unequal_and_same_type', 0); </pre>

sbioselect

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

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

Conditions for Properties Names or String Values	Example Syntax
<p>regex. Supports expressions supported by the functions <code>regex</code> and <code>regexpi</code>.</p>	<p>Search in the model object (<code>modelObj</code>), and return objects that have 'ese' or 'ase' anywhere within the name.</p> <pre>Obj = sbioselect (modelObj, 'Where',... 'Name', 'regex', '[ea]se')</pre> <p>Search in the root, and return objects that have kinase anywhere within the name.</p> <pre>Obj = sbioselect ('Where',... 'Name', 'regex', 'kinase')</pre> <p>Note that this query could result in a mixture of object types (for example, species and parameters).</p>
<p><code>regexpi</code></p>	<p>Same as <code>regex</code>; in addition, this is case insensitive.</p>
<p><code>~regex</code></p>	<p>Search in the model object (<code>modelObj</code>), and return objects that do not have kinase anywhere within the name.</p> <pre>Obj = sbioselect (modelObj, 'Where',... 'Name', '~regex', 'kinase')</pre>
<p><code>~regexpi</code></p>	<p>Same as <code>~regex</code>; in addition, this is case insensitive.</p>
<p><code>wildcard</code></p>	<p>Supports DOS-style wildcards ('?' matches any single character, '*' matches any number of characters, and the pattern must match the entire string). See <code>regexptranslate</code> for more information.</p>
<p><code>wildcardi</code></p>	<p>Same as <code>wildcard</code>; in addition, this is case insensitive.</p>

sbioselect

Conditions for Properties Names or String Values	Example Syntax
-wildcard	Search in the model object (modelObj), and return objects that have names that do not begin with kin*. <pre>Obj = sbioselect (modelObj, 'Where', ... 'Name', '~wildcard', 'kin*')</pre>
-wildcardi	Same as -wildcard; in addition, this is case insensitive.

Use the condition type function for any property. The specified value should be a function handle that, when applied to a property value, returns a boolean indicating whether there is a match. The following table shows an example of using function.

Condition	Example Syntax
'function'	<p>Search in the model object and return reaction objects whose Stoichiometry property contains the specified stoichiometry.</p> <pre> Out = sbioselect(modelObj, 'Where', ... 'Stoichiometry', 'function', ... @(x)any(x>2)) </pre> <p>Select all objects with a numeric value that is even.</p> <pre> iseven = @(x) isnumeric(x)... && isvector(x) && mod(x, 2) == 0; evenValuedObj = sbioselect(modelObj, ... 'where', 'Value', 'function', iseven); </pre>

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

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

```

Out = sbioselect(Obj, 'Where', 'PropertyName1', 'Condition1',
PropertyValue1, 'Where', 'PropertyName2', 'Condition2',

```

PropertyValue2,...) finds objects contained by *Obj* that matches all the conditions specified.

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

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

Examples

- 1 Import a model.

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

- 2 Find and return an object named pA.

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

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

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

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

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

SimBiology Species Array

Index:	Compartment:	Name:	InitialAmount:	InitialAmountUnits:
1	unnamed	pB	0	

- 5 Find and return objects that do not have their units set.

```
unitlessObj = sbioselect(modelObj, 'Where', 'wildcard', '*Units', '==', '');  
%Alternatively,  
unitlessObj = sbioselect(modelObj, '*Units', '');
```

See Also `regex`

sbiosetdosingprofile

Purpose Add objects to model for dosing

Note `sbiosetdosingprofile` has been removed and produces an error. Use `sbiodose` and `adddose` instead.

Syntax

```
modModelObj = sbiosetdosingprofile(modelObj, DoseVariable,  
                                DosingTable, DosingType)
```

Arguments

<i>modModelObj</i>	Modified model object containing dosing information, returned by <code>sbiosetdosingprofile</code> .
<i>modelObj</i>	SimBiology model object to which you want to add dosing information.
<i>DoseVariable</i>	Name of a species or parameter object in <i>modelObj</i> . <code>sbiosetdosingprofile</code> adds events that change the amount or value of the <i>DoseVariable</i> as defined by the <i>DosingTable</i> and <i>DosingType</i> .
<i>DosingTable</i>	An nx2 matrix with the first column defining the time of the dose and the second column defining the dose amount. If <i>DosingType</i> is 'Infusion', then <i>DosingTable</i> must be nx3 with a third column that defines the rate of infusion.
<i>DosingType</i>	Specifies the mechanism for drug dosing. Valid options are 'Bolus', 'Infusion', 'ZeroOrder', 'FirstOrder' and ''. For more information on <i>DosingType</i> see in the SimBiology User's Guide.

Description

```
modModelObj = sbiosetdosingprofile(modelObj, DoseVariable,  
                                DosingTable, DosingType)
```

 adds SimBiology event and rule objects to the model object *modelObj* to perform the dosing as specified by

DoseVariable, *DosingTable*, and *DosingType* and returns the modified model object, *modModelObj*.

While SimBiology performs dimensional checks and unit conversions for components in a model, it does not handle units for quantities in *DosingTable*. For more information about units in *DosingTable*, see in the SimBiology User's Guide.

To facilitate the removal of the modified components from the model object, *sbiosetdosingprofile* adds the keyword 'DOSE_COMPONENT' to the Tag property for the events and the associated parameters added to the model object, *modelObject*.

To remove the modified components from the modified model object, *modModelObject*, use `delete(sbioselect(modModelObject, 'Tag', 'DOSE_COMPONENT'))`;

Model Components Added by sbiosetdosingprofile

sbiosetdosingprofile adds the following model components based on the dosing type you selected.

In the parameter names below, the suffix '_n' denotes a numeric suffix that gives each parameter a unique name. The first dosing parameter is named with the suffix '_1', the second with '_2', and so on.

For all dosing types *sbiosetdosingprofile* adds a parameter, *DosingGroupID* that causes dosing rules and events to be evaluated only when the parameter value is 1.

Bolus:

- A parameter, *BolusDoseAsAmount_n*, that represents the time of the doses.
- For a dose at time = 0
 - An initial assignment rule that increases the initial drug concentration (by default = 0), by the sum of all doses occurring at time = 0, divided by the compartment volume.
- For doses at time > 0

sbiosetdosingprofile

- A parameter for all doses occurring at time, $BolusDoseTime_n$, that represents the time of the doses.
- An event at $BolusDoseTime_n$ that increases the drug concentration by the sum of all doses occurring at that dose time.

Infusion:

- A parameter named $InfusionRateChange_n$ with a value equal to the infusion rate.
- A second parameter named $InfusionRateChange_n$ with a value equal to the negative of the infusion rate; used to end the infusion dose.
- For a dose at time = 0
 - An initial assignment rule to increase the parameter representing the rate of infusion (k_{Inf}) by the sum of all doses occurring at time = 0.
- For doses starting or ending at time > 0
 - A parameter, $InfusionChangeTime_n$, that represents time of the dose changes occurring at the same time. The start of a dose is the time listed in *DosingTable*. The end of a dose is $InfusionChangeTime_n + \text{amount/rate of infusion}$. Amount and rate are values specified in the second and third columns respectively of *DosingTable*.
 - An event at $InfusionChangeTime_n$ that changes the value of k_{Inf} by the sum of all dose changes occurring at this time.

Zero-order:

Note For custom models, include a parameter named $Tk0$, representing the duration of drug absorption.

- A parameter, `ZeroOrderDoseStart_n`, with a value equal to the amount of the dose.
- A second parameter, `ZeroOrderDoseEnd_n` with a value equal to the negative of the amount of the dose; used to end the dose.
- If doses start at time = 0
 - An initial assignment rule to increase the parameter representing the absorption rate constant (k_a) by the sum of all doses occurring at time = 0, divided by Tk_0 .
- If doses start at time > 0
 - A parameter, `ZeroOrderDoseStartTime_n`, that represents the start of the dose. This value is defined in the first column of *DosingTable*.
 - An event at `ZeroOrderDoseStartTime_n` that increases the parameter representing the absorption rate constant (k_a) by the sum of all doses starting at this time, divided by Tk_0 .
- For the end of all doses, which occurs at time > 0
 - A parameter `ZeroOrderDoseEndTime_n` that is used to end the dose and has a value equal to the dose start time. (Because the numerical value depends on the parameter Tk_0 , it cannot be set explicitly to the actual end time.)
 - An event occurring at time `ZeroOrderDoseEndTime_n + Tk_0` that decreases the parameter representing the absorption rate constant (k_a) by the sum of all doses ending at this time, divided by Tk_0

First-order:

- For each dose, a parameter, `FirstOrderDoseAmount_n`, that holds the dose amount for the current dose.
- For a dose at time = 0
 - An initial assignment rule that increases `Dose` by the sum of all doses occurring at time = 0.

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- For each dose at time > 0
 - A parameter for all doses occurring at this time, `FirstOrderDoseTime_n`, that represents the time of the dose.
 - A parameter, `FirstOrderDoseAmount_n`, that holds amount of the dose.
 - An event at `FirstOrderDoseTime_n` that increases the value of `Dose` by the sum of all doses occurring at that dose time.

See Also

`sbiodose` and `adddose`

Purpose Show unit prefixes in library

Syntax

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

Arguments

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

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

`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*.

sbioshowunitprefixes

`[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

`sbioconvertunits`, `sbioshowunits`, `sbiunitprefix`

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

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

sbioshowunits

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

`sbioconvertunits`, `sbioshowunitprefixes`, `sbiunit`

Purpose

Simulate model object

Syntax

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

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 2-130.

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*, *doseObj*) simulates a model object (*modelObj*), using the dose object or array of dose objects (*doseObj*).

... = 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*).

Input Arguments

modelObj

SimBiology model object.

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.

doseObj

Specify the dose object to apply to the model during the simulation. For more information about dose objects, see `ScheduleDose` object and `RepeatDose` object.

Output Arguments

t

An n -by-1 vector of time points. Shows the simulation time steps.

x

An n -by- m data array, where n is the number of time samples and m is the number of states logged in the simulation. Each column of x describes the variation in the quantity of a state over time.

names

An m -by-1 cell array of names. If the species are in multiple compartments, species names are qualified with the compartment name in the form `compartmentName.speciesName`. For example, `nucleus.DNA`, `cytoplasm.mRNA`.

Parameter names are qualified with the reaction name if the parameter is scoped to the reaction's kinetic law. For example,

Transcription.k1, denotes that the parameter k1 is scoped to the kinetic law for the reaction Transcription.

simdataObj

An object that holds time and state data as well as metadata, such as the types and names for the logged states or the configuration set used during simulation. You can access time, data, and names stored in *simdataObj* through *simdataObj* properties. See `SimData` object for more information.

Examples

The following examples show 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 sundials), 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 ode23s and set StopTime to 10.

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

- 4 Simulate the modelObj.

```
[t,x]= sbiosimulate(modelObj);
```

- 5 Plot the results of the simulation.

```
plot(t, x)
```

Example 2

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

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

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

- 2 Simulate the `modelObj`.

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

- 3 Plot the results of the simulation.

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

See Also

`addconfigset` | `sbioaccelerate` | `sbiomodel`

Purpose Construct species object

Note sbiospecies has been removed and produces an error. Use addspecies instead.

Syntax

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

Arguments

<i>NameValue</i>	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.
<i>InitialAmountValue</i>	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 the species object name (*NameValue*).

In order for a species object to be used in a simulation, you must add the species object 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.

Species names are automatically updated for reactions that use the `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
get (any object)	Get object properties
rename (compartment, parameter, species)	Rename object and update expressions
set (any object)	Set object properties

Property Summary

Properties for species object

Annotation	Store link to URL or file
BoundaryCondition	Indicate species boundary condition
ConstantAmount	Specify variable or constant species amount
InitialAmount	Species initial amount
InitialAmountUnits	Species initial amount units
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
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 named H2O and an initial amount of 1000.

```
speciesObj = sbiospecies('H2O', 1000);  
% View the help for the species object's InitialAmount property.  
help(speciesObj, 'InitialAmount')
```

- 2 View properties for the species object.

```
get(speciesObj)  
    Annotation: ''  
    BoundaryCondition: 0  
    ConstantAmount: 0  
    InitialAmount: 1000  
    InitialAmountUnits: ''  
    Name: 'H2O'  
    Notes: ''  
    Parent: []  
    Tag: ''  
    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 named glucose_6_phosphate and glucose_6_phosphate_dehydrogenase.


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

- 2 Set the initial amount of glucose_6_phosphate to 100 and verify.

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

MATLAB returns:

```
ans =  
  
    100
```

See Also

`addspecies`

MATLAB functions `get`, `set`

sbiosubplot

Purpose Plot simulation results in subplots

Syntax

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

Arguments

<i>simDataObj</i>	SimBiology data object.
<i>fcnHandleValue</i>	Function handle.
<i>xArgsValue</i>	Cell array with the names of the states.
<i>yArgsValue</i>	Cell array with the names of the states.
<i>showLegendValue</i>	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 the SimBiology data object, *simDataObj*, into its own subplot. The subplot is plotted by calling the function handle, *fcnHandleValue*, with input arguments *simDataObj*, *xArgsValue*, and *yArgsValue*.

`sbiosubplot(simDataObj, fcnHandleValue, xArgsValue, yArgsValue, showLegendValue)` plots each simulation run for the SimBiology data 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 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 = sbioensamplerun(m1, 10, 'linear');
sbiosubplot(simDataObj);
```

See Also sbioplot

Purpose

Plot simulation results in trellis plot

Syntax

```
trellisplot = sbiotrellis(Dataset, GroupCol, XCol, YCol)  
trellisplot = sbiotrellis(Dataset, GroupCol, XCol, YCol, ...)  
trellisplot = sbiotrellis(Dataset, fcnHandleValue, GroupCol,  
    XCol, YCol)  
trellisplot = sbiotrellis(simDataObj, fcnHandleValue, XCol,  
    YCol)
```

Arguments

<i>trellisplot</i>	Object returned by <code>sbiotrellis</code> . Use <code>trellisplot</code> together with the <code>plot</code> method to overlay trellis plots. See “Description” on page 2-140 for information about the <code>plot</code> method.
<i>Dataset</i>	dataset containing grouped data to plot.
<i>GroupCol</i>	Column containing groups.
<i>Xcol</i>	Data column to plot on x-axis.
<i>YCol</i>	Data column to plot on y-axis.
<i>fcnHandleValue</i>	Function handle. If '' (empty), default is <code>@plot</code> .
<i>simDataObj</i>	SimBiology data object.

Description

`trellisplot = sbiotrellis(Dataset, GroupCol, XCol, YCol)` plots each group in *Dataset* by the data column *GroupCol* into its own subplot. The data defined by column *XCol* is plotted against the data defined by column *YCol*.

`trellisplot = sbiotrellis(Dataset, GroupCol, XCol, YCol, ...)` takes optional property/value pairs that are supported by the `plot` command. Refer to `plot` in the MATLAB Reference documentation for more information on available properties.

`trellisplot = sbiotrellis(Dataset, fcnHandleValue, GroupCol, XCol, YCol)` plots each group in *Dataset* as defined by the data column *GroupCol* into its own subplot. `sbiotrellis` creates the subplot by calling the function handle, *fcnHandleValue*, with input arguments defined by the *Dataset* columns *XCol* and *YCol*.

`trellisplot = sbiotrellis(simDataObj, fcnHandleValue, XCol, YCol)` plots each group in the *SimData* object (*simdataObj*) into its own subplot. `sbiotrellis` creates the subplot by calling the function handle, *fcnHandleValue* with input arguments defined by the columns *XCol* and *YCol*.

Use the `plot` method to overlay a *SimData* object or a dataset on an existing `sbiotrellis` plot. The command, `plot(trellisplot, ...)` adds a plot to the trellis plot defined by the `sbiotrellis` object, `trellisplot`. The *SimData* or dataset object that is being plotted must have the same number of elements/groups as the trellis plot. The `plot` method has the same input arguments as `sbiotrellis`. For an example, see “Performing Population Fitting Using `sbionlmefit` or `sbionlmefitsa`” in the *SimBiology* documentation.

See Also

`sbioplot`, `sbiosubplot`

Purpose Create user-defined unit

Syntax

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

Arguments

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

<i>PropertyName</i>	Name of the unit object property, for example, 'Notes'.
<i>PropertyValue</i>	Value of the unit object property, for example, 'New unit for GPCR model'.

Description

unitObject = `sbiounit('NameValue')` constructs a SimBiology unit object named *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

`sbioaddtolibrary`, `sbishowunits`, `sbiunitprefix`, `sbiowhos`

sbiunitcalculator

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

Purpose Create user-defined unit prefix

Syntax

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

Arguments

<i>NameValue</i>	Name of the user-defined unit prefix. <i>NameValue</i> must begin with characters and can contain characters, underscores, or numbers. <i>NameValue</i> can be any valid MATLAB variable name.
<i>ExponentValue</i>	Shows the value of 10^{Exponent} that defines the relationship of the unit <i>Name</i> to the base unit. For example, for the unit picomole, Exponent is 12.
<i>PropertyName</i>	Name of the unit prefix object property. For example, 'Notes'.
<i>PropertyValue</i>	Value of the unit prefix object property. For example, 'New unitprefix for GPCR model'.

Description

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

unitprefixObject = `sbiunitprefix('NameValue', 'ExponentValue')` creates a unit-prefix object with a multiplicative factor of $10^{\text{ExponentValue}}$.

unitprefixObject = `sbiunitprefix('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).

sbiounitprefix

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 `sbiowhowsunitprefixes` function to list the units available in the user-defined library.

Examples

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

- 1 Create a unit prefix.

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

- 2 Add the unit prefix 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

sbiaddtolibrary, sbioshowunits, sbiunit, sbiowhos

sbiounregisterunit

Purpose Remove user-defined unit from root and library

Note `sbiounregisterunit` has been removed and produces an error. 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`, `sbiounit`, `sbiowhos`

Purpose Remove user-defined unit prefix from root and library

Note sbionregisterunitprefix has been removed and produces an error. Use sbioremovefromlibrary instead.

Syntax sbionregisterunitprefix('Name')

Description sbionregisterunitprefix('Name') removes the user-defined unit prefix with the name *Name* from the user-defined library. You cannot remove a unit prefix from the built-in library. If *Name* is a user-defined unit prefix, it is removed from the UserDefinedUnits vector on the SimBiology root object and also from the user library. Once unregistered, this unit prefix is not available in future MATLAB sessions. You can list the available unit prefixes and find information on whether the unit prefix is built in or user defined using sbiowhos or sbioshowunitprefixes.

See Also sbioremovefromlibrary, sbioroot, sbioshowunitprefixes, sbiunitprefix, sbiowhos

sbiupdate

Purpose Update SimBiology model version

Syntax
`modelsObj = sbiupdate(modelObj)`
`simdataObj = sbiupdate(tsObj)`

Arguments

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

Description

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

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

Arguments

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

Description

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

variantObj = sbiovariant('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.

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

Method Summary

<code>addcontent</code> (variant)	Append content to variant object
<code>commit</code> (variant)	Commit variant contents to model
<code>copyobj</code> (any object)	Copy SimBiology object and its children
<code>delete</code> (any object)	Delete SimBiology object
<code>display</code> (any object)	Display summary of SimBiology object
<code>get</code> (any object)	Get object properties
<code>rmcontent</code> (variant)	Remove contents from variant object
<code>set</code> (any object)	Set object properties
<code>verify</code> (model, variant)	Validate and verify SimBiology model

Property Summary

<code>Active</code>	Indicate object in use during simulation
<code>Annotation</code>	Store link to URL or file
<code>Content</code>	Contents of variant object
<code>Name</code>	Specify name of object
<code>Notes</code>	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 object that varies the InitialAmount property of a species named A.

```
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 kinetic laws, units, and unit prefixes.

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

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

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

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

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

Examples

```
% Show contents of the SimBiology root object
sbiowhos
```

```
% Show 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 kinetic laws from a library file.
sbiowhos -kineticlaw mylibraryfile

% Show all contents of multiple files.
sbiowhos myfile1 myfile2
```

See AlsoMATLAB 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 a Systems Biology Markup Language (SBML) format. Enter either a file name or a path and file name supported by your operating system. If the file name does not have the extension `.xml`, then `.xml` is appended to end of the file name.

Description

`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 the SimBiology Getting Started Guide for more information.

Example

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

```
sbmlexport(modelObj, 'gene_regulation.xml');
```

Reference

Finney, A., Hucka, M., (2003), *Systems Biology Markup Language (SBML) Level 2: Structures and facilities for model definitions*. Accessed from SBML.org

See Also `sbiomodel`, `sbiosaveproject`, `sbmlimport`

sbmlimport

Purpose Import SBML-formatted file

Syntax `modelObj = sbmlimport('FileName')`

Description `modelObj = sbmlimport('FileName')` imports a Systems Biology Markup Language (SBML) formatted file named *FileName* into MATLAB and creates a model object `modelObj`. *FileName* extensions are `.sbml` or `.xml`. Enter either a file name or a path and file name supported by your operating system. `sbmlimport` supports SBML Levels 1 and Level 2 Version 1.

For functional characteristics and limitations, see “SBML Support” in the SimBiology Getting Started Guide documentation.

Examples Import SBML model:

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

References Finney, A., Hucka, M., (2003). *Systems Biology Markup Language (SBML) Level 2: Structures and facilities for model definitions*. SBML.org.

Alternatives Use the SimBiology desktop:

1 In the MATLAB Command Window, type:

```
simbiology
```

The SimBiology desktop opens.

2 Select **File > New Project**. The New Project Wizard opens.

3 Add data using the **Add Data** pane, or click **Next**.

4 In the **Add Model** pane, from the **Select a model to add** list, select **Load model from file**

5 Browse to or specify the name of the project or SBML file.

6 Click **Next**.

7 In the **Choose Analysis** pane, select the analysis tasks to add to the model and click **Finish**.

A new project with the selected specifications opens.

See Also

`get` | `sbiosimulate` | `sbmlexport` | `set`

Purpose Open SimBiology modeling and simulation GUI

Syntax
`simbiology`
`simbiology(modelObj)`

Arguments

<i>modelObj</i>	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 `simbiology` opens the SimBiology desktop, which lets you do the following:

- Build a SimBiology model by representing reaction pathways and entering 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 through individual or ensemble runs.
- View results from the simulation.
- Perform analysis tasks such as sensitivity analysis, parameter and species scans, and calculate conserved moieties.
- Create and/or modify user-defined units and unit prefixes.
- Create and/or modify user-defined kinetic laws.

`simbiology(modelObj)` opens the SimBiology desktop with a top-level SimBiology model object (*modelObj*). If there is a project open in the SimBiology desktop, this command adds the model (*modelObj*) to the project. A top-level SimBiology model object has its property `Parent` set to the SimBiology root object. Thus, querying `sbioroot` at the command

line shows you all models in the MATLAB workspace, including the models available in the desktop. Any changes you make to the model at the command line are reflected in the desktop because both are pointing to the same model object in the `Root` object.

Note The `sbioreset` command removes all models from the root object and therefore this command also removes all models from the SimBiology desktop.

Examples

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

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

See Also

`sbioroot`

simbiology

Method Reference

Objects (p. 3-3)	SimBiology objects
Abstract Kinetic Laws (p. 3-4)	Work with abstract kinetic law objects
Compartments (p. 3-5)	Work with compartment objects
Configuration Sets (p. 3-6)	Work with configuration set objects
Events (p. 3-6)	Work with event objects
Kinetic Laws (p. 3-7)	Create parameter objects and work with kinetic law objects
Models (p. 3-8)	Create SimBiology objects and work with model objects
Parameters (p. 3-11)	Work with parameter objects
Pharmacokinetic Modeling (p. 3-12)	Create and work with objects for PK modeling and analysis
Reactions (p. 3-13)	Create kinetic law and species objects and work with reaction objects
RepeatDose (p. 3-13)	Methods for RepeatDose objects
Root (p. 3-14)	Work with the root object
Rules (p. 3-15)	Work with rule objects
ScheduleDose (p. 3-15)	Methods for ScheduleDose objects
SimData (p. 3-16)	Methods for SimData objects
Species (p. 3-17)	Methods for species objects
Units and Unit Prefixes (p. 3-17)	Methods for unit and prefix objects

Variants (p. 3-17)

Using Object Methods (p. 3-19)

Methods for variant objects

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
PKCompartment object	Used by PKModelDesign to create SimBiology model
PKData object	Define roles of data set columns
PKModelDesign object	Helper object to construct pharmacokinetic model
PKModelMap object	Define SimBiology model components roles
Reaction object	Options for model reactions
RepeatDose object	Define drug dosing protocol
Root object	Hold models, unit libraries, and abstract kinetic law libraries
Rule object	Hold rule for species and parameters
ScheduleDose object	Define drug dosing protocol
SimData object	Simulation data storage
Species object	Options for compartment species
Unit object	Hold information about user-defined unit
UnitPrefix object	Hold information about user-defined unit prefix
Variant object	Store alternate component values

Abstract Kinetic Laws

delete (any object)

display (any object)

get (any object)

set (any object)

Delete SimBiology object

Display summary of SimBiology
object

Get object properties

Set object properties

Compartments

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

Configuration Sets

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

Events

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

Kinetic Laws

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

Models

<code>addcompartment (model, compartment)</code>	Create compartment object
<code>addconfigset (model)</code>	Create configuration set object and add to model object
<code>adddose (model)</code>	Add dose object to model
<code>addevent (model)</code>	Add event object to model object
<code>addparameter (model, kineticlaw)</code>	Create parameter object and add to model or kinetic law object
<code>addreaction (model)</code>	Create reaction object and add to model object
<code>addrule (model)</code>	Create rule object and add to model object
<code>addvariant (model)</code>	Add variant to model
<code>copyobj (any object)</code>	Copy SimBiology object and its children
<code>delete (any object)</code>	Delete SimBiology object
<code>display (any object)</code>	Display summary of SimBiology object
<code>get (any object)</code>	Get object properties
<code>getadjacencymatrix (model)</code>	Get adjacency matrix from model object
<code>getconfigset (model)</code>	Get configuration set object from model object
<code>getdose (model)</code>	Return SimBiology dose object
<code>getstoichmatrix (model)</code>	Get stoichiometry matrix from model object
<code>getvariant (model)</code>	Get variant from model
<code>removeconfigset (model)</code>	Remove configuration set from model
<code>removedose (model)</code>	Add dose object to model

<code>removevariant (model)</code>	Remove variant from model
<code>reorder (model, compartment)</code>	Reorder component lists
<code>set (any object)</code>	Set object properties
<code>setactiveconfigset (model)</code>	Set active configuration set for model object
<code>verify (model, variant)</code>	Validate and verify SimBiology model

Parameters

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

Pharmacokinetic Modeling

addCompartment (PKModelDesign)	Add compartment to PKModelDesign object
construct (PKModelDesign)	Construct SimBiology model from PKModelDesign object
get (any object)	Get object properties
PKCompartment object	Used by PKModelDesign to create SimBiology model
PKData object	Define roles of data set columns
PKModelDesign object	Helper object to construct pharmacokinetic model
PKModelMap object	Define SimBiology model components roles
set (any object)	Set object properties

Reactions

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

RepeatDose

copyobj (any object)	Copy SimBiology object and its children
get (any object)	Get object properties
set (any object)	Set object properties

Root

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

Rules

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

ScheduleDose

copyobj (any object)	Copy SimBiology object and its children
get (any object)	Get object properties
set (any object)	Set object properties

SimData

delete (any object)	Delete SimBiology object
display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
getdata (SimData)	Get data from SimData object array
getsensmatrix (SimData)	Get 3-D sensitivity matrix from SimData array
resample (SimData)	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
set (any object)	Set object properties

Species

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

Units and Unit Prefixes

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

Variants

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

display (any object)

Display summary of SimBiology
object

get (any object)

Get object properties

rmcontent (variant)

Remove contents from variant object

set (any object)

Set object properties

verify (model, variant)

Validate and verify SimBiology
model

Using Object Methods

Command-line syntax for using methods with SimBiology objects

Constructing (Creating) Objects
(p. 3-19)

Using Object Methods (p. 3-19)

Help for Objects, Methods, and
Properties (p. 3-20)

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 referenced by a reaction, use the reaction object methods `addkineticlaw`, `addparameter`, `addproduct`, and `addreactant`.

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

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

Using Object Methods

Using MATLAB function notation:

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

Using object dot notation:

ObjectName.MethodName(arguments, ...)

Help for Objects, Methods, and Properties

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

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

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 a *kinetic law definition*, 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 kinetic law definition specifies 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 kinetic law definition relates to the kinetic law object, see `KineticLaw` object.

Create your own kinetic law definition and add it to the kinetic law library with the `sbioaddtolibrary` function. You can then use the kinetic law to define a reaction rate. To retrieve a kinetic law definition from the user-defined library, use the command `get(sbioroot, 'UserDefinedKineticLaws')`.

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

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

Constructor Summary

<code>sbioabstractkineticlaw</code>	Create kinetic law definition
-------------------------------------	-------------------------------

Method Summary

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

Property Summary

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 kinetic law definition
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

<i>modelObj</i>	Model object.
<i>owningCompObj</i>	Compartment object that contains the newly created compartment object.
<i>NameValue</i>	Name for a compartment object. Enter a character string unique to the model object. For information on naming compartments, see Name.
<i>CapacityValue</i>	Capacity value for the compartment object. Enter double. Positive real number, default = 1.
<i>PropertyName</i>	Enter the name of a valid property. Valid property names are listed in “Property Summary” on page 4-6.
<i>PropertyValue</i>	Enter the value for the property specified in <i>PropertyName</i> . 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.

addcompartment (model, compartment)

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

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

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

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

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

addcompartment (model, compartment)

Method Summary

Methods for compartment objects

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

Property Summary

Properties for compartment objects

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

addcompartment (model, compartment)

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	

addcompartment (model, compartment)

- 5 Display the Compartments property in the compartment object.

```
get(compartmentObj2, 'Compartments')
```

```
SimBiology Compartment - matrix
```

```
Compartment Components:
```

```
Capacity:          1
```

```
CapacityUnits:
```

```
Compartments:     0
```

```
ConstantCapacity: true
```

```
Owner:            mitochondrion
```

```
Species:          0
```

See Also

addproduct, addreactant, addreaction, addspecies, get, set

addCompartment (PKModelDesign)

Purpose Add compartment to PKModelDesign object

Syntax `PKCompartmentObj = addCompartment(PKModelDesignObj, Name, 'DosingType', 'EliminationType', HasResponseVariable)`

Arguments **Input Arguments**

PKModelDesignObj The PKModelDesign object to which you want to add a compartment

Name Name of the compartment object that is constructed

DosingType Specifies the mechanism for drug absorption. Valid options are 'Bolus', 'Infusion', 'ZeroOrder', 'FirstOrder' and ''. You can only specify one compartment in a model with a dosing type other than '' (empty). For more information on *DosingType*, see “About Dosing Types” in the SimBiology documentation

EliminationType Specifies the mechanism for drug elimination. Valid options are 'Linear', 'Linear-Clearance', 'Enzymatic', and ''. For more information on *EliminationType*, see “About Elimination Types” in the SimBiology documentation.

HasResponseVariable Logical indicating if the drug concentration in this compartment is reported. Only one compartment can have this set to true.

Output Arguments

PKCompartmentObj PKCompartment object

Description `PKCompartmentObj = addCompartment(PKModelDesignObj, Name, 'DosingType', 'EliminationType', HasResponseVariable)` adds a

addCompartment (PKModelDesign)

compartment with the specified name, dosing and elimination type, and specifies whether the compartment contains a measured (or observed) response.

Method Summary

get (any object)	Get object properties
set (any object)	Set object properties

Property Summary

DosingType	Drug dosing type in compartment
EliminationType	Drug elimination type from compartment
HasResponseVariable	Compartment drug concentration reported
Name	Specify name of object

See Also

“Creating PK Models at the Command Line”, PKCompartment object
PKModelDesign object

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 in “Property Summary” on page 4-12.

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*.

addconfigset (model)

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

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

Property Summary

Properties for configuration set objects

<code>Active</code>	Indicate object in use during simulation
<code>CompileOptions</code>	Dimensional analysis and unit conversion options
<code>Name</code>	Specify name of object
<code>Notes</code>	HTML text describing SimBiology object
<code>RuntimeOptions</code>	Options for logged species
<code>SensitivityAnalysisOptions</code>	Specify sensitivity analysis options
<code>SolverOptions</code>	Specify model solver options
<code>SolverType</code>	Select solver type for simulation
<code>StartTime</code>	Start time for simulation or initial dose time
<code>StopTime</code>	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: 'sundials'  
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);
```

addconfigset (model)

`plot (t,x)`

See Also

`get, getconfigset, removeconfigset, set, setactiveconfigset`

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

addcontent (variant)

Description

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

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

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

Examples

1 Create a model containing one species.

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

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

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

See Also

`addvariant`, `rmcontent`, `sbiovariant`

Purpose Add dose object to model

Syntax

```
doseObj2 = adddose(mode1Obj, 'DoseName')  
doseObj2 = adddose(mode1Obj, 'DoseName', 'DoseType')  
doseObj2 = adddose(mode1Obj, doseObj)
```

Arguments

<i>mode1Obj</i>	Model object to which you add a dose object.
<i>DoseName</i>	Name of a dose object to construct and add to a model object. <i>DoseName</i> is the value of the dose object property Name.
<i>DoseType</i>	Type of dose object to construct and add to a model object. Enter either 'schedule' or 'repeat'.
<i>doseObj</i>	Dose object to add to a model object. Created with the constructor sbiodose.

Outputs

<i>doseObj2</i>	ScheduleDose or RepeatDose object. A RepeatDose or ScheduleDose object defines an increase (dose) to a species amount during a simulation.
-----------------	--

Description

Before using a dose object in a simulation, use the `adddose` method to add the dose object to a SimBiology model object. Then, set the `Active` dose object property to `true`.

`doseObj2 = adddose(mode1Obj, 'DoseName')` constructs a SimBiology RepeatDose object (`doseObj2`), assigns `DoseName` to the property `Name`, adds the dose object to a SimBiology model object (`mode1Obj`), and assigns `mode1Obj` to the property `Parent`.

adddose (model)

`doseObj2 = adddose(modelObj, 'DoseName', 'DoseType')` constructs either a SimBiology ScheduleDose object or RepeatDose object (`doseObj`).

`doseObj2 = adddose(modelObj, doseObj)` adds a SimBiology dose object (`doseObj`) to a SimBiology model object (`modelObj`), copies the dose object to a second dose object (`doseObj2`), and assigns `modelObj` to the property `Parent`.

Example

Add a dose object to a model object.

- 1 Create a model then add a dose to the model.

```
modelObj = sbiomodel('mymodel');  
dose1Obj = adddose(modelObj, 'dose1');
```

- 2 Define properties of the dose object.

```
dose1Obj.Amount = 5;  
dose1Obj.Repeat = 6;  
dose1Obj.Interval = 24;  
dose1Obj.TimeUnits = 'hour'
```

See Also

Model object methods:

- `adddose` — add a dose object to a model object
- `getdose` — get dose information from a model object
- `removedose` — remove a dose object from a model object

Dose object constructor `sbiodose`.

ScheduleDose object and RepeatDose object methods:

- `copyobj` — copy a dose object from one model object to another model object
- `get` — view properties for a dose object

- `set` — define or modify properties for a dose object

addevent (model)

Purpose Add event object to model object

Syntax

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

Arguments

<i>modelObj</i>	Model object.
<i>TriggerValue</i>	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 <code>Trigger</code> for more information.
<i>EventFcnsValue</i>	A string or a cell array of strings, each of which specifies an assignment of the form ' <i>objectname</i> = <i>expression</i> ', where <i>objectname</i> is the name of a valid object. Defines what occurs when the event is triggered. See <code>EventFcns</code> for more information.
<i>PropertyName</i>	Property name for an event object from “Property Summary” on page 4-21.
<i>PropertyValue</i>	Property value. For more information on property values, see the property reference for each property listed in “Property Summary” on page 4-21.

Description

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

When the trigger expression in the property `Trigger` changes from false to true, the assignments in `EventFcns` are executed during simulation.

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

`eventObj = addevent(...'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

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

Property Summary

<code>Active</code>	Indicate object in use during simulation
<code>Annotation</code>	Store link to URL or file
<code>EventFcns</code>	Event expression
<code>Name</code>	Specify name of object
<code>Notes</code>	HTML text describing SimBiology object

addevent (model)

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

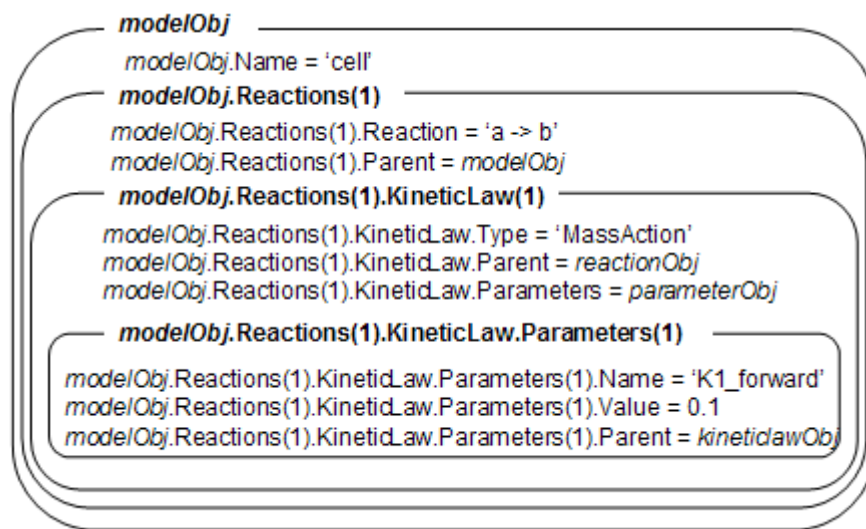
<i>reactionObj</i>	Reaction object. Enter a variable name for a reaction object.
<i>KineticLawNameValue</i>	Property to select the type of kinetic law object to create. For built-in kinetic law, valid values are: 'Unknown', 'MassAction', 'Henri-Michaelis-Menten', 'Henri-Michaelis-Menten-Reversible',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

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 kinetic law definition. See “Kinetic Law Definition” on page 6-61 for a definition of 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

addkineticlaw (reaction)

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 in “Property Summary” on page 4-27.

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

<code>addparameter (model, kineticlaw)</code>	Create parameter object and add to model or kinetic law object
<code>copyobj (any object)</code>	Copy SimBiology object and its children
<code>delete (any object)</code>	Delete SimBiology object
<code>display (any object)</code>	Display summary of SimBiology object
<code>get (any object)</code>	Get object properties
<code>getparameters (kineticlaw)</code>	Get specific parameters in kinetic law object
<code>getspecies (kineticlaw)</code>	Get specific species in kinetic law object
<code>set (any object)</code>	Set object properties
<code>setparameter (kineticlaw)</code>	Specify specific parameters in kinetic law object
<code>setspecies (kineticlaw)</code>	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 kinetic law definition
Parent	Indicate parent object
SpeciesVariableNames	Cell array of species 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

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.

addkineticlaw (reaction)

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

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

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

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

The `addkineticlaw` method adds a kinetic law to the reaction object (*reactionObj*).

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

- 3** Add parameter objects to a kinetic law object. For example, create a parameter object `parameterObj1` named `Vm_d`, another parameter object (`parameterObj2`) named `Km_d`, and add them to a kinetic law object (`kineticlawObj`).

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

The `addparameter` method creates two parameter objects with values that are associated with the kinetic law parameters.

- 4** Associate kinetic law parameters with the parameters in the kinetic law definition.

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

This method associates the parameters in the property `ParameterVariableNames` with the 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.

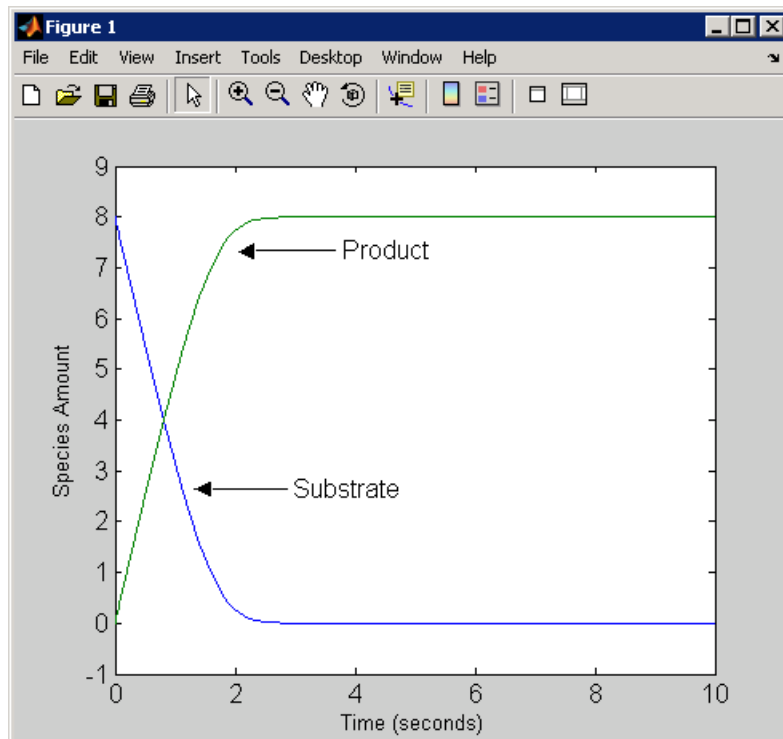
```
get (reactionObj, 'ReactionRate')

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)
```

addkineticlaw (reaction)



Example 2

This example uses the built-in kinetic law MassAction.

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

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

- 2 Define a kinetic law for the reaction object.

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

MassAction

Notice, the property Expression for MassAction kinetic law does not show the parameters and species in the reaction rate.

- 3 Assign the rate constant for the reaction.

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

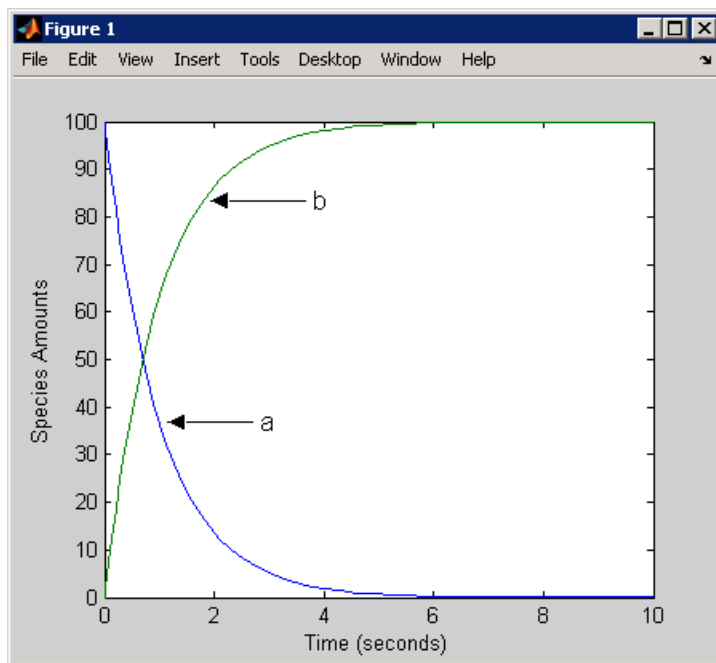
```
ans =  
    k_forward*a
```

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

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

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

addkineticlaw (reaction)



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 sbiupdate to convert submodels into models.

Syntax

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

Arguments

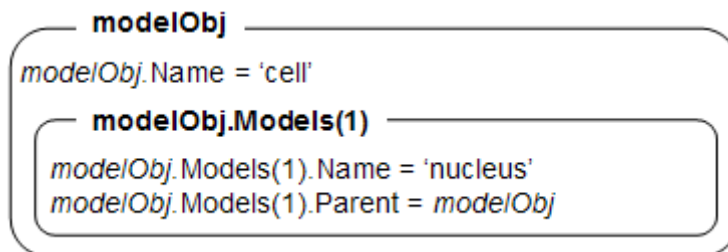
<i>modelObj</i>	Model object. Enter a name for a model object.
<i>NameValue</i>	Descriptive name for a model object. Enter a unique character string. A model object can be referenced by other objects using this property.
<i>submodelObj</i>	Model object to be added as a submodel.

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')
```

addmodel (model)



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`, `sbiouupdate`

addparameter (model, kineticlaw)

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

<i>Obj</i>	Model or kinetic law object. Enter a variable name for the object.
<i>NameValue</i>	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. For information on naming parameters, see Name.
<i>ValueValue</i>	Property for a parameter object. Enter a number.

Description

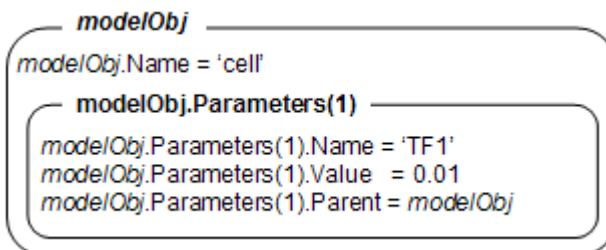
`parameterObj = addparameter(Obj, 'NameValue')` creates a parameter object and returns the object (*parameterObj*). In the parameter object, this method assigns a value (*NameValue*) to the property Name, assigns a value 1 to the property Value, and assigns the model or kinetic law object to the property 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

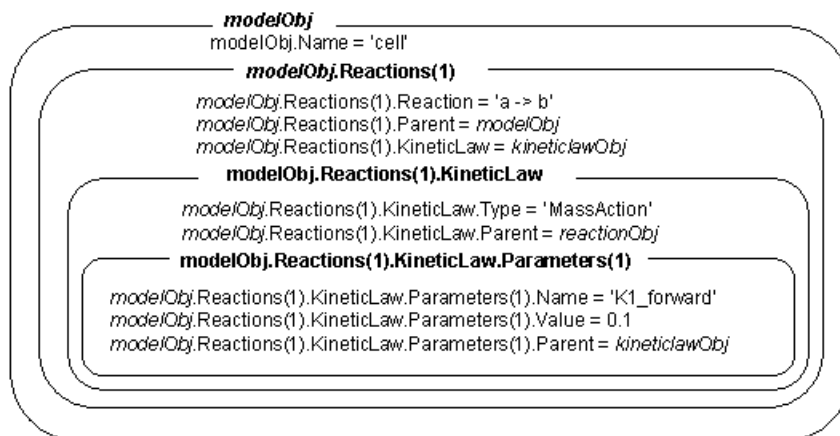
addparameter (model, kineticlaw)

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)
```



addparameter (model, kineticlaw)

`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
get (any object)	Get object properties
rename (compartment, parameter, species)	Rename object and update expressions
set (any object)	Set object properties

Property Summary

Properties for parameter objects

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

addparameter (model, kineticlaw)

Example

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

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

- 2 Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

- 3 Add a parameter and assign it to the kinetic law object (kineticlawObj); 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

<i>reactionObj</i>	Reaction object. Enter a name for the reaction object.
<i>NameValue</i>	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 <code>sbioselect</code> to find an object with a specific <i>NameValue</i> .
<i>speciesObj</i>	Species object.
<i>Stoichcoefficient</i>	Stoichiometric coefficients for products, length of array equal to length of <i>NameValue</i> , or length of <i>speciesObj</i> .

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`.

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

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

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

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

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

addproduct (reaction)

uses the new name. You must however configure all other applicable elements such as rules that use the species, and the kinetic law object.

Examples

- 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

addspecies, sbiospecies

Purpose

Add species object as reactant to reaction object

Syntax

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

Arguments

<i>reactionObj</i>	Reaction object.
<i>NameValue</i>	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 <code>sbioselect</code> to find an object with a specific Name property value.
<i>speciesObj</i>	Species object or cell array of species objects.
<i>Stoichcoeffieient</i>	Stoichiometric coefficients for reactants, length of array equal to length of <i>NameValue</i> or length of <i>speciesObj</i> .

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.

addreactant (reaction)

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

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

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

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

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

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

See for more information on species names.

Example

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

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

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

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

See Also

addspecies, sbiospecies

addraction (model)

Purpose

Create reaction object and add to model object

Syntax

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

Arguments

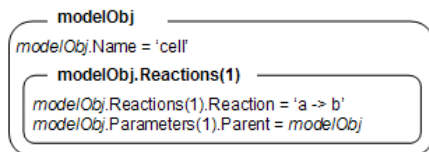
<i>modelObj</i>	SimBiology model object.
<i>ReactionValue</i>	<p>Specify the reaction equation. Enter a character string. A hyphen preceded by a space and followed by a right angle bracket (->) indicates reactants going forward to products. A hyphen with left and right angle brackets (<->) indicates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

<i>ReactantsValue</i>	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.
<i>ProductsValue</i>	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.
<i>RStoichCoefficients</i>	Stoichiometric coefficients for reactants, length of array equal to length of <i>ReactantsValue</i> .
<i>PStoichCoefficients</i>	Stoichiometric coefficients for products, length of array equal to length of <i>ProductsValue</i> .

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:

addreaction (model)

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

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

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

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

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

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

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


`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

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

addreaction (model)

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, and then add a reaction object.

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

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

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

reactionObj.KineticLaw property is configured to kineticlawObj.

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

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

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

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

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

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

MATLAB returns:

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

See Also

addkineticlaw, addproduct, addreactant, rmproduct, rmreactant

addrule (model)

Purpose Create rule object and add to model object

Syntax

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

Arguments

<i>modelObj</i>	Model object to which to add the rule.
<i>RuleValue</i>	Enter a character string within quotation marks. For example, enter the algebraic rule 'Va*Ea + Vi*Ei - K2'.
<i>RuleTypeValue</i>	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

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

Property Summary

Properties for rule objects

<code>Active</code>	Indicate object in use during simulation
<code>Annotation</code>	Store link to URL or file
<code>Name</code>	Specify name of object
<code>Notes</code>	HTML text describing SimBiology object
<code>Parent</code>	Indicate parent object
<code>Rule</code>	Specify species and parameter interactions
<code>RuleType</code>	Specify type of rule for rule object
<code>Tag</code>	Specify label for SimBiology object

addrule (model)

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

Examples

Add a rule with the default RuleType.

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

```
modelObj = sbiomodel('cell');  
ruleObj = addrule(modelObj, '0.1*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: '0.1*B-A'  
RuleType: 'algebraic'  
Tag: ''  
Type: 'rule'  
UserData: []
```

Add a rule with the RuleType property set to rate.

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

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

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

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

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

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

MATLAB returns all the properties for the rule object.

```
Active: 1  
Annotation: ''  
Name: ''  
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

<i>compObj</i>	Compartment object.
<i>NameValue</i>	Name for a species object. Enter a character string unique within <i>compObj</i> . Species objects are identified by name within <i>Event</i> , <i>ReactionRate</i> , and <i>Rule</i> property strings. For information on naming species, see <i>Name</i> . You can use the function <i>sbiiselect</i> to find an object with a specific <i>Name</i> property value.
<i>InitialAmountValue</i>	Initial amount value for the species object. Enter <i>double</i> . Positive real number, default = 0.
<i>PropertyName</i>	Enter the name of a valid property. Valid property names are listed in “Property Summary” on page 4-58.
<i>PropertyValue</i>	Enter the value for the property specified in <i>PropertyName</i> . 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*.

addspecies (compartment)

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

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

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

addspecies (compartment)

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

Species names are automatically updated for reactions that use `MassAction` kinetic law.

Method Summary

Methods for species objects

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

Property Summary

Properties for species objects

<code>Annotation</code>	Store link to URL or file
<code>BoundaryCondition</code>	Indicate species boundary condition
<code>ConstantAmount</code>	Specify variable or constant species amount
<code>InitialAmount</code>	Species initial amount
<code>InitialAmountUnits</code>	Species initial amount units
<code>Name</code>	Specify name of object
<code>Notes</code>	HTML text describing SimBiology object
<code>Parent</code>	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, where one is a reactant and the other is the enzyme catalyzing the reaction.

- 1 Create a model object named `my_model` and add a compartment object.

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

- 2 Add two species objects named `glucose_6_phosphate` and `glucose_6_phosphate_dehydrogenase`.

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

- 3 Set the 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(modelObj, 'Species')
```

addspecies (compartment)

MATLAB returns:

```
SimBiology Species Array
```

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

5 Retrieve information about the first species in the array.

```
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, get, set

Purpose Add variant to model

Syntax

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

Arguments

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

Description

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

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.

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

addvariant (model)

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 the `InitialAmount` property of a species named A.

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

See Also

`addcontent`, `commit`, `copyobj`, `delete`, `getvariant`

Purpose Commit variant contents to model

Syntax `commit(variantObj, modelObj)`

Arguments

<i>modelObj</i>	Specify the model object to which you want to commit a variant.
<i>variantObj</i>	Variant object to commit to the 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 replace 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 the `InitialAmount` property of a species named A.

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

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

commit (variant)

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

See Also addvariant, Variant 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 object

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 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 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 4-67 for links to compartment property reference pages. Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

`addcompartment` (model, compartment)

Create compartment object

Method Summary

Methods for compartment objects

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

Property Summary

Properties for compartment objects

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

Compartment 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

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 4-70 for links to configset object property reference pages.

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

Constructor Summary

`addconfigset (model)`

Create configuration set object and add to model object

Configset object

Method Summary

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

Property Summary

Active	Indicate object in use during simulation
CompileOptions	Dimensional analysis and unit conversion options
Name	Specify name of object
Notes	HTML text describing SimBiology object
RuntimeOptions	Options for logged species
SensitivityAnalysisOptions	Specify sensitivity analysis options
SolverOptions	Specify model solver options
SolverType	Select solver type for simulation
StartTime	Start time for simulation or initial dose time
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

construct (PKModelDesign)

Purpose Construct SimBiology model from PKModelDesign object

Syntax `[modelObj, pkModelMapObject] = construct(pkModelDesignObject)`

Arguments

<i>modelObj</i>	SimBiology model object specifying a pharmacokinetic model.
<i>pkModelMapObject</i>	Defines the roles of the components in <i>modelObj</i> . See PKModelMap object for more information.

Description

`[modelObj, pkModelMapObject] = construct(pkModelDesignObject)` constructs a SimBiology model object containing the model components (such as compartments, species, reactions, and rules) required to represent a pharmacokinetic model specified in `pkModelDesignObject`. The newly constructed model object is named 'Generated Model' (which you can change).

See Also

in the SimBiology User's Guide, PKModelDesign 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, species, or variant object.

parentObj

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

modelObj Model object to be copied.

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

Description

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

copyobj (any object)

`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`.

When the `copyobj` method copies a model, it resets the `StatesToLog` property to the default value. Similarly, the `SpeciesInputFactors` and `ParameterInputFactors` are not copied but rather left empty. Thus, when you simulate a copied model you see results for the default states, unless you manually update these properties.

Examples

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

- 1 Create a model object and add a reaction object.

```
modelObj1 = sbiomodel('cell');  
reactionObj = addreaction(modelObj1, 'a -> b');
```

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

```
modelObj2 = sbiomodel('cell2');  
reactionObjCopy = copyobj(reactionObj, modelObj2);  
modelObj2.Reactions
```

SimBiology Reaction Array

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

See Also

`sbiomodel`, `sbioroot`

Purpose Delete SimBiology object

Syntax `delete(Obj)`

Arguments

Obj abstract kinetic law, configuration set, event, kinetic law, model, parameter, reaction, rule, SimData, species, unit, unit prefix, or variant object.

Description

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

- If *Obj* is a model object, the model is deleted from the root object. `delete` removes all references to the model both at the command line and in the SimBiology desktop.
- 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 that you cannot delete the default configuration set.
- You cannot delete the SimBiology root.

delete (any object)

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`

Purpose Display summary of SimBiology object

Syntax `display(Obj)`

Arguments

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

Description

Display the SimBiology object array. `display(Obj)` is called for the SimBiology object, *Obj* when the semicolon is not used to terminate a statement. The display of *Obj* gives a brief summary of the *Obj* configuration. You can view a complete list of *Obj* properties with the command `get`. You can modify all *Obj* properties that can be changed, with the command `set`.

Examples

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

Event object

Purpose Store event information

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

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

See “Property Summary” on page 4-79 for links to event property reference pages.

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

Constructor Summary

<code>addevent (model)</code>	Add event object to model object
-------------------------------	----------------------------------

Method Summary

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

Property Summary

Active	Indicate object in use during simulation
Annotation	Store link to URL or file
EventFcns	Event expression
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Tag	Specify label for SimBiology object
Trigger	Event trigger
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, Species object

get (any object)

Purpose Get object properties

Syntax
PropertyValue = get(*Obj*, '*PropertyName*')
objProperties = get(*Obj*)

Arguments

PropertyValue Value defined for '*PropertyName*'

Obj Abstract kinetic law, compartment, configuration set, event, kinetic law, model, parameter, PKCompartment, PKData, PKModelDesign, PKModelMap, reaction, rule, SimData, species, or variant object.

'*PropertyName*' Name of the property to get.

objProperties Struct containing properties and values for the object, *Obj*.

Description *PropertyValue* = get(*Obj*, '*PropertyName*') gets the value '*PropertyValue*' of the object, *Obj*'s *PropertyName* property.

objProperties = get(*Obj*) gets the properties for the object, *Obj*, and returns it to *objProperties*.

Examples 1 Create a model object.

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


2 Add parameter object.

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

3 Set the ConstantValue property of the parameter object to false and verify.

MATLAB returns 1 for true and 0 for false.

```
set (parameterObj, 'ConstantValue', false);  
get(parameterObj, 'ConstantValue')
```

MATLAB returns

```
ans =
```

```
0
```

See Also

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

getadjacencymatrix (model)

Purpose Get adjacency matrix from model object

Syntax

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

Arguments

<i>M</i>	Adjacency matrix for <i>modelObj</i> .
<i>modelObj</i>	Specify the model object.
<i>Headings</i>	Return row and column headings. If species are in multiple compartments, species names are qualified with the compartment name in the form <code>compartmentName.speciesName</code> . For example, <code>nucleus.DNA</code> , <code>cytoplasm.mRNA</code> .
<i>Mask</i>	Return 1 for the species object and 0 for the reaction object to <i>Mask</i> .

Description

`getadjacencymatrix` returns the adjacency matrix for a model object.

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

An adjacency matrix is defined by listing all species contained by *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, Headings] = getadjacencymatrix(modelObj)` 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 1s and 0s 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`

getConfigset (model)

Purpose Get configuration set object from model object

Syntax

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

Arguments

<i>modelObj</i>	Model object. Enter a variable name for a model object.
<i>NameValue</i>	Name of the configset object.
<i>configsetObj</i>	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 the name configured to 'default'. Additional configset objects can be added to *modelObj* with the method addconfigset.

Examples

1 Retrieve the default configset object from the modelObj.

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

```
Configuration Settings - default (active)
  SolverType:      sundials
  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

getdata (SimData)

Purpose Get data from SimData object array

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

Arguments Output Arguments

<i>t</i>	An n-by-1 vector of time points.
<i>x</i>	An n-by-m data array. <i>t</i> and <i>names</i> label the rows and columns of <i>x</i> respectively.
<i>names</i>	An m-by-1 cell array of names.
<i>Metadata</i>	When used with the 'nummetadata' input argument, <i>Metadata</i> contains a cell array of metadata structures. The elements of <i>Metadata</i> label the columns of <i>x</i> .
<i>Out</i>	Data returned in the format specified in 'FormatValue', shown in "Input Arguments" on page 4-86. Depending on the specified 'FormatValue', <i>Out</i> contains one of the following: <ul style="list-style-type: none">• Structure array• SimData object• Time series object• Combined time series object from an array of SimData objects

Input Arguments

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

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

getdata (SimData)

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 <code>simDataObj</code> .
'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 4-86.

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.

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

- 2 Get all the simulation data from the SimData object.

```
[t x names] = getdata(simDataObj);
```


Retrieving Data for Ensemble Runs

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

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

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

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

- 3 Get all the simulation data from the `SimData` object.

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

See Also

`display`, `get`, `resample`, `selectselectbyname`, `setactiveconfigset`
MATLAB function struct

getdose (model)

Purpose Return SimBiology dose object

Syntax

```
doseObj = getdose(modelObj)
doseObj = getdose.modelObj
doseObj = getdose(modelObj, 'DoseName')
```

Arguments

modelObj Selects a model object that contains a dose object.

DoseName Name of a dose object contained in a model object. *DoseName* is from the dose object property, Name.

Outputs

doseObj ScheduleDose or RepeatDose object retrieved from a model object. A RepeatDose or ScheduleDose object defines an increase (dose) to a species amount during a simulation.

Description

doseObj = getdose(*modelObj*) or *doseObj* = getdose.modelObj returns a Simbiology dose object (*doseObj*) contained in a Simbiology model object (*modelObj*).

doseObj = getdose(*modelObj*, 'DoseName') returns a SimBiology dose object (*modelObj*) with the name *DoseName*.

Examples

Get a dose object from a model object.

- 1 Create a model object, and then add a dose object to the model object.

```
modelObj = sbiomodel('mymodel');
dose1Obj = adddose(modelObj, 'dose1');
```

- 2 Get the dose object from a model object.

```
myModelDose = getdose(modelObj);
```

See Also

Model object methods:

- `adddose` — add a dose object to a model object
- `getdose` — get dose information from a model object
- `removedose` — remove a dose object from a model object

Dose object constructor `sbiodose`.

`ScheduleDose` object and `RepeatDose` object methods:

- `copyobj` — copy a dose object from one model object to another model object
- `get` — view properties for a dose object
- `set` — define or modify properties for a dose object

getparameters (kineticlaw)

Purpose Get specific parameters in kinetic law object

Syntax

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

Arguments

<i>kineticlawObj</i>	Retrieve parameters used by the kinetic law object.
<i>ParameterVariablesValue</i>	Retrieve parameters used by the kinetic law object corresponding to the specified parameter in the <code>ParameterVariables</code> 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`.

Examples

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

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

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

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

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

- 3 Add two parameter objects.

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

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

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

- 5 To retrieve a parameter variable:

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

MATLAB returns:

```
SimBiology Parameter Array
```

Index:	Name:	Value:	ValueUnits:
1	Va	1	

```
parameterObj4 = getparameters(kineticlawObj, 'Km')
```

See Also

addparameter, getspecies, setparameter

getsensmatrix (SimData)

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

<i>T</i>	<i>T</i> is an <i>m</i> -by-1 array specifying time points for the sensitivity data in <i>R</i> .
<i>R</i>	<i>R</i> is an <i>m</i> -by- <i>n</i> -by- <i>p</i> array of sensitivity data with times, outputs, and input factors corresponding to its first, second, and third dimensions respectively. <i>R</i> (:, <i>i</i> , <i>j</i>) is the time course for the sensitivity of state <i>Outputs</i> { <i>i</i> } to the input factor <i>InputFactors</i> { <i>j</i> }.
<i>Outputs</i>	Name of the output factors, where output factors are the names of the states for which you want to calculate sensitivity.
<i>InputFactors</i>	Name of the 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 documentation 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.

getsensmatrix (SimData)

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

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

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

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

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

- e** Enable `SensitivityAnalysis`.

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

```
ans =
```

```
1
```

- f** Simulate and return the results in a `SimData` object.

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

- 2** Extract and plot sensitivity data from the `SimData` object.

- a** Use `getsensmatrix` to retrieve sensitivity data.

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

- b** Plot sensitivity values.

```
plot(t, R(:,:,2));
legend(outs);
```



```
title(['Sensitivities of species relative to ' ifacs{2}]);
```

See Also

display, get, getdata, resample, selectbyname

MATLAB function struct

getspecies (kineticlaw)

Purpose Get specific species in kinetic law object

Syntax

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

Arguments

<i>kineticlawObj</i>	Retrieve species used by the kinetic law object.
<i>SpeciesVariablesValue</i>	Retrieve species used by the kinetic law object corresponding to the specified species in the <code>SpeciesVariables</code> 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, the reaction updates 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`.

Examples

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

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

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

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

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

reactionObj KineticLaw property is configured to kineticlawObj.

- 3 The 'Henri-Michaelis-Menten' kinetic law has 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, getparameters, setparameter, setspecies

getstoichmatrix (model)

Purpose Get stoichiometry matrix from model object

Syntax

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

Arguments

<i>M</i>	Adjacency matrix for <i>modelObj</i> .
<i>modelObj</i>	Specify the model object <i>modelObj</i> .
<i>objSpecies</i>	Return the list of <i>modelObj</i> species by Name property of the species. If the species are in multiple compartments, species names are qualified with the compartment name in the form <code>compartmentName.speciesName</code> . For example, <code>nucleus.DNA</code> , <code>cytoplasm.mRNA</code> .
<i>objReactions</i>	Return the list of <i>modelObj</i> reactions by the Name property of reactions.

Description `getstoichmatrix` returns a stoichiometry matrix for a model object.

`M = getstoichmatrix(modelObj)` returns a stoichiometry matrix for a SimBiology 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 $2 A + B \rightarrow 3 C$ and $B + 3 D \rightarrow 4 A$, the stoichiometry matrix would be defined as:

	A	B	C	D
R1	-2	-1	3	0
R2	4	-1	0	-3

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

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

Examples

- 1 Read in a model using `sbmlimport`.

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

- 2 Get the stoichiometry matrix for the `modelObj`.

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

See Also

`getadjacencymatrix`

getvariant (model)

Purpose Get variant from model

Syntax
`variantObj = getvariant(modelObj)`
`variantObj = getvariant(modelObj, 'NameValue')`

Arguments

<code>variantObj</code>	Variant object returned by the <code>getvariant</code> method.
<code>modelObj</code>	Model object from which to get the variant.
<code>'NameValue'</code>	Name of the variant to get from the model object <code>modelObj</code> .

Description

`variantObj = getvariant(modelObj)` returns SimBiology variant objects contained by the SimBiology model object `modelObj` to `variantObj`.

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see [Variant object](#).

`variantObj = getvariant(modelObj, 'NameValue')` returns the SimBiology variant object with the name `NameValue`, contained by the SimBiology model object, `modelObj`.

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

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

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`

KineticLaw object

Purpose Kinetic law information for reaction

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

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

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

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

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

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

For links to kinetic law object property reference pages, see “Property Summary” on page 4-109.

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

For an explanation of how relevant properties relate to one another, see “Command Line” on page 4-105.

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:

$$V_m * S / (K_m + S)$$

In the SimBiology software 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 SimBiology Getting Started Guide documentation.

Command Line

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

```
A -> B
where Vm = Va, Km = Ka
```

KineticLaw object

and $S = A$

Define V_a and K_a in the `ParameterVariableNames` property to substitute the variables that are in the `ParameterVariables` property (V_m and K_m). 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  $V_m = V_a$ 
%  $V_m$  is listed first in 'ParameterVariables',
% therefore list  $V_a$  first in 'ParameterVariableNames'.

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

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

$$V_a * A / (K_a + A)$$

For a detailed procedure, see “Examples” on page 4-110.

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

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

KineticLaw object

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

Constructor Summary

addkineticlaw (reaction)

Create kinetic law object and add to reaction object

Method Summary

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

Property Summary

Annotation	Store link to URL or file
Expression	Expression to determine reaction rate equation
KineticLawName	Name of kinetic law applied to reaction
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parameters	Array of parameter objects

KineticLaw object

ParameterVariableNames	Cell array of reaction rate parameters
ParameterVariables	Parameters in kinetic law definition
Parent	Indicate parent object
SpeciesVariableNames	Cell array of species 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.

- 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 the names Va and Ka, and then add them to kineticlawObj. The species object with Name A is created when reactionObj is created and need not be redefined.

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

- 5 Set the variable names for the kinetic law object.

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

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

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

MATLAB returns:

```
ans =

    Va*A/(Ka+A)
```

See Also

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

SimBiology property Expression

Model object

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 4-114 for links to model property reference pages.

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

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

Constructor Summary

<code>sbiomodel</code>	Construct model object
------------------------	------------------------

Method Summary

<code>addcompartment (model, compartment)</code>	Create compartment object
--	---------------------------

<code>addconfigset (model)</code>	Create configuration set object and add to model object
-----------------------------------	---

<code>adddose (model)</code>	Add dose object to model
------------------------------	--------------------------

<code>addevent (model)</code>	Add event object to model object
-------------------------------	----------------------------------

<code>addparameter (model, kineticlaw)</code>	Create parameter object and add to model or kinetic law object
---	--

<code>addreaction (model)</code>	Create reaction object and add to model object
<code>addrule (model)</code>	Create rule object and add to model object
<code>addvariant (model)</code>	Add variant to model
<code>copyobj (any object)</code>	Copy SimBiology object and its children
<code>delete (any object)</code>	Delete SimBiology object
<code>display (any object)</code>	Display summary of SimBiology object
<code>get (any object)</code>	Get object properties
<code>getadjacencymatrix (model)</code>	Get adjacency matrix from model object
<code>getconfigset (model)</code>	Get configuration set object from model object
<code>getdose (model)</code>	Return SimBiology dose object
<code>getstoichmatrix (model)</code>	Get stoichiometry matrix from model object
<code>getvariant (model)</code>	Get variant from model
<code>removeconfigset (model)</code>	Remove configuration set from model
<code>removedose (model)</code>	Add dose object to model
<code>removevariant (model)</code>	Remove variant from model
<code>reorder (model, compartment)</code>	Reorder component lists
<code>set (any object)</code>	Set object properties

Model object

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

Purpose

Parameter and scope information

Description

The parameter object represents a *parameter*, which is a quantity that can change or can be constant. SimBiology parameters are generally used to define rate constants. You can add parameter objects to a model object or a kinetic law object. The scope of a parameter depends on where you add the parameter object: If you add the parameter object to a model object, the parameter is available to all reactions in the model and the Parent property of the parameter object is `SimBiology.Model`. If you add the parameter object to a kinetic law object, the parameter is available only to the reaction for which you are using the kinetic law object and the Parent property of the parameter object is `SimBiology.KineticLaw`.

See “Property Summary” on page 4-116 for links to parameter object property reference pages.

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

Constructor Summary

<code>addparameter (model, kineticlaw)</code>	Create parameter object and add to model or kinetic law object
---	--

Method Summary

<code>copyobj (any object)</code>	Copy SimBiology object and its children
<code>delete (any object)</code>	Delete SimBiology object
<code>display (any object)</code>	Display summary of SimBiology object
<code>get (any object)</code>	Get object properties

Parameter object

rename (compartment, parameter, species)	Rename object and update expressions
set (any object)	Set object properties

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 object, KineticLaw object, Model object, Reaction object, Root object, Rule object, Species object

Purpose

Used by PKModelDesign to create SimBiology model

Description

The PKCompartment object is used by the PKModelDesign object to construct a SimBiology model for pharmacokinetic modeling. PKCompartment holds the following information:

- Name of the compartment
- Dosing type
- Elimination type
- Whether the drug concentration in this compartment is reported

The PKCompartment class is a subclass of the hgsetget class which is a subclass of the handle class. For more information on the inherited methods, see hgsetget, and handle.

Construction

addCompartment
(PKModelDesign)

Add compartment to
PKModelDesign object

Method Summary

get (any object)

Get object properties

set (any object)

Set object properties

Property Summary

DosingType

Drug dosing type in compartment

EliminationType

Drug elimination type from
compartment

HasResponseVariable

Compartment drug concentration
reported

Name

Specify name of object

PKCompartment object

See Also in the SimBiology User's Guide, PKModelDesign object

Purpose

Define roles of data set columns

Description

The properties of the PKData object specify what each column in the data represents. The PKData object specifies which columns in the data set represent the following:

- The grouping variable
- The independent and dependent variables
- The dose
- The rate (only if infusion is the dosing type)
- The covariates

This information is used by the fitting functions, `sbionlmefit` and `sbionlinfit`.

To create the PKData object specify:

```
pkDataObject = PKData(data);
```

Where `data` is the imported data set.

The PKData class is a subclass of the `hgsetget` class, which is a subclass of the `handle` class. For more information on the inherited methods, see `hgsetget` and `handle`.

Construction

PKData

Create PKData object

Method Summary

get (any object)

Get object properties

set (any object)

Set object properties

PKData object

Property Summary

CovariateLabels	Identify covariate columns in data set
DataSet	Dataset object containing imported data
DependentVarLabel	Identify dependent variable column in data set
DependentVarUnits	Response units in PKData object
DoseLabel	Dose column in data set
DoseUnits	Dose units in PKData object
GroupID	Integer identifying each group in data set
GroupLabel	Identify group column in data set
GroupNames	Unique values from GroupLabel in data set
IndependentVarLabel	Identify independent variable column in data set
IndependentVarUnits	Time units in PKData object
RateLabel	Rate of infusion column in data set
RateUnits	Units for dose rate

See Also

in the SimBiology User's Guide, PKModelDesign object

Purpose

Helper object to construct pharmacokinetic model

Description

Use the `PKModelDesign` object to construct a `SimBiology` model for PK modeling. The `PKModelDesign` object lets you specify the number of compartments, the type of dosing, and method of elimination which you then use to construct the `SimBiology` model object with the necessary compartments, species, reactions, rules, and events.

```
pkm = PKModelDesign;
```

Use the `addCompartment` method to add a compartment with a specified dosing and elimination. `addCompartment` adds each subsequent compartment and connects it to the previous compartment using a reversible reaction. This reaction models the flux between compartments in a PK model.

The `construct` method uses the `PKModelDesign` object to create a `SimBiology` model object.

The `PKModelDesign` class is a subclass of the `hgsetget` class, which is a subclass of the `handle` class. For more information on the inherited methods see `hgsetget` and `handle`.

Construction

`PKModelDesign`

Create `PKModelDesign` object

Method Summary

`addCompartment`
(`PKModelDesign`)

Add compartment to
`PKModelDesign` object

`construct` (`PKModelDesign`)

Construct `SimBiology` model from
`PKModelDesign` object

`get` (any object)

Get object properties

`set` (any object)

Set object properties

PKModelDesign object

Property Summary

PKCompartments

Hold compartments in PK model

See Also

“Creating PK Models at the Command Line”, PKCompartment object

Purpose	Define SimBiology model components roles										
Description	<p>The PKModelMap object holds information about the dosing type, and defines which components of a SimBiology model represent the observed response, the dose, and the estimated parameters.</p> <p>The PKModelMap class is a subclass of the hgsetget class which is a subclass of the handle class. For more information on the inherited methods see, hgsetget, and handle.</p>										
Construction	<table><tr><td>PKModelMap</td><td>Create PKModelMap object</td></tr></table>	PKModelMap	Create PKModelMap object								
PKModelMap	Create PKModelMap object										
Method Summary	<table><tr><td>get (any object)</td><td>Get object properties</td></tr><tr><td>set (any object)</td><td>Set object properties</td></tr></table>	get (any object)	Get object properties	set (any object)	Set object properties						
get (any object)	Get object properties										
set (any object)	Set object properties										
Property Summary	<table><tr><td>Dosed</td><td>Dosed object name</td></tr><tr><td>DosingType</td><td>Drug dosing type in compartment</td></tr><tr><td>Estimated</td><td>Names of parameters to estimate</td></tr><tr><td>Observed</td><td>Measured response object name</td></tr><tr><td>ZeroOrderDurationParameter</td><td>Zero order dose absorption duration</td></tr></table>	Dosed	Dosed object name	DosingType	Drug dosing type in compartment	Estimated	Names of parameters to estimate	Observed	Measured response object name	ZeroOrderDurationParameter	Zero order dose absorption duration
Dosed	Dosed object name										
DosingType	Drug dosing type in compartment										
Estimated	Names of parameters to estimate										
Observed	Measured response object name										
ZeroOrderDurationParameter	Zero order dose absorption duration										
See Also	“Defining Model Components for Observed Response, Dose, Dosing Type, and Estimated Parameters” in the SimBiology User’s Guide, PKModelDesign 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 + phosphocreatine`

`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 4-125 for links to reaction object property reference pages.

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

Constructor Summary

<code>addreaction (model)</code>	Create reaction object and add to model object
----------------------------------	--

Method Summary

<code>addkineticlaw (reaction)</code>	Create kinetic law object and add to reaction object
<code>addproduct (reaction)</code>	Add product species object to reaction object
<code>addreactant (reaction)</code>	Add species object as reactant to reaction object
<code>copyobj (any object)</code>	Copy SimBiology object and its children
<code>delete (any object)</code>	Delete SimBiology object

display (any object)	Display summary of SimBiology object
get (any object)	Get object properties
rmproduct (reaction)	Remove species object from reaction object products
rmreactant (reaction)	Remove species object from reaction object reactants
set (any object)	Set object properties

Property Summary

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

Reaction 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, Root object, Rule object, Species object

Purpose Remove configuration set from model

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

Arguments

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

Description

`removeconfigset(modelObj, 'NameValue')` removes the configset object with the name *NameValue* from the SimBiology model object *modelObj*. A configuration set object stores simulation-specific information. A SimBiology model can contain multiple configuration sets with one being active at any given time. The active configuration set contains the settings that are used during the simulation. *modelObj* always contains at least one configuration set object with name configured to 'default'. You cannot remove the default configuration set from *modelObj*. If the active configuration set is removed from *modelObj*, then the default configuration set will be made active.

`removeconfigset(modelObj, configsetObj)` removes the configuration set object, *configsetObj*, from the 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.

Examples

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

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

removeconfigset (model)

```
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 Add dose object to model

Syntax
`doseObj2 = removedose(modelObj, 'DoseName')`
`doseObj2 = removedose(modelObj, doseObj)`

Arguments

<i>modelObj</i>	Model object from which you remove a dose object.
<i>DoseName</i>	Name of the dose object to remove from a model object. <i>DoseName</i> is the value of the dose object property Name.
<i>doseObj</i>	Dose object to remove from a model object.

Outputs

<i>doseObj2</i>	ScheduleDose or RepeatDose object.
-----------------	------------------------------------

Description

`doseObj2 = removedose(modelObj, 'DoseName')` removes a SimBiology ScheduleDose or RepeatDose object with the name *DoseName* from a model object (*modelObj*). returns the dose object (*doseObj*), and assigns [] to the dose object property Parent.

You can add a removed dose object back to a model object using the method `adddose`.

`doseObj2 = removedose(modelObj, doseObj)` removes a SimBiology ScheduleDose or RepeatDose object *doseObj*.

Examples

Remove a dose object from a model object.

- 1 Create model and dose objects, and then add dose to model.

```
modelObj = sbiomodel('mymodel');  
doseObj = adddose(modelObj, 'dose1');
```

- 2 Remove dose object from model object.

removedose (model)

```
removedose(mymodel, 'dose1');
```

Get all dose objects from a model object, and then remove the second dose object.

```
AllDoseObjects = getdose(mymodel);  
removedose(mymodel, AllDoseObjects(2));
```

See Also

Model object methods:

- `adddose` — add a dose object to a model object
- `getdose` — get dose information from a model object
- `removedose` — remove a dose object from a model object

Dose object constructor `sbiodose`.

`ScheduleDose` object and `RepeatDose` object methods:

- `copyobj` — copy a dose object from one model object to another model object
- `get` — view properties for a dose object
- `set` — define or modify properties for a dose object

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 the variant.

variantObj Specify the variant object to return from the model object.

Description

variantObj = removevariant(*modelObj*, 'NameValue') removes a SimBiology variant object with the name *NameValue* from the model object *modelObj* and returns the variant object to *variantObj*. The variant object *Parent* property is assigned [] (empty).

A SimBiology variant object stores alternate values for properties on a SimBiology model. For more information on variants, see [Variant object](#).

variantObj = removevariant(*modelObj*, *variantObj*) removes a SimBiology variant object (*variantObj*) and 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 (model)

```
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

rename (compartment, parameter, species)

Purpose Rename object and update expressions

Syntax `rename(Obj, 'NewNameValue')`

Arguments

Obj Compartment, parameter, or species object.

'*NewNameValue*' Specify the new name.

Description

`rename(Obj, 'NewNameValue')`, changes the Name property of the object, *Obj* to *NewNameValue* and updates any expressions in the model (such as Rule or ReactionRate) to use the new name.

If the new name is already being used by another model component, the new name will be qualified to ensure that it is unique. For example if you change a species named A to K, and a parameter with the name K exists, the species will be qualified as *CompartmentName.K* to indicate that the reference is to the species. If you are referring to an object by its qualified name, for example *CompartmentName.A* and you change the species name, the reference will contain the qualified name in its updated form, for example, *CompartmentName.K*

When you want to change the name of a compartment, parameter, or species object, use this method instead of `set`. The `set` method only changes the Name property of the object, except for species objects where the species object's Name property and any reaction strings which refer to species are updated to use the new name.

Examples

- 1 Create a model object that contains a species A in a rule.

```
m = sbiomodel('cell');
s = addspecies(m, 'A');
r = addrule(m, 'A = 4');
```

- 2 Rename the species to Y

```
rename(s, 'Y');
```

rename (compartment, parameter, species)

3 See that the rule expression is now updated.

```
r
```

```
SimBiology Rule Array
```

```
Index:      RuleType:      Rule:
1           initialAssignment  Y = 4
```

See Also set

reorder (model, compartment)

Purpose Reorder component lists

Syntax `modelObj = reorder(Obj, NewOrder)`

Arguments

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

Description

`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
```

reorder (model, compartment)

3 Reverse the order of the reactions in the model.

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


Purpose

Define drug dosing protocol

Description

A `RepeatDose` object defines a series of doses to the amount of a species during a simulation. The `TargetName` property of a dose object defines the species that receives the dose.

Each dose is the same amount, as defined by the `Amount` property, and given at equally spaced times, as defined by the `Interval` property. The `RepeatCount` property defines the number of injections in the series, excluding the initial injection. The `Rate` property defines how fast each dose is given.

To use a dose object in a simulation you must add the dose object to a model object and set the `Active` property of the dose object to true. Set the `Active` property to true if you always want the dose to be applied before simulating the model.

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

See “Property Summary” on page 4-184 for links to species property reference pages. Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

`sbiodose`

Construct dose object

RepeatDose object

Method Summary

Methods for RepeatDose objects

copyobj (any object)	Copy SimBiology object and its children
get (any object)	Get object properties
set (any object)	Set object properties

Property Summary

Properties for RepeatDose objects

Active	Indicate object in use during simulation
Amount	Amount of dose
AmountUnits	Dose amount units
Annotation	Store link to URL or file
DurationParameterName	Specify parameter with length of time
Interval	Amount of dose
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rate	Amount of dose
RateUnits	Units for dose rate
RepeatCount	Dose repetitions
StartTime	Start time for simulation or initial dose time
Tag	Specify label for SimBiology object
TargetName	Species receiving dose

TimeUnits	Show stop time units for simulation
Type	Display top-level SimBiology object type
UserData	Specify data to associate with object

See Also

Model object, ScheduleDose object, sbiodose, sbiosimulate

resample (SimData)

Purpose Resample SimData object array onto new time vector

Syntax

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

Arguments

<i>newSimDataObj</i>	Resampled SimData object array.
<i>simDataObj</i>	SimData object array that you want to resample.
<i>timevector</i>	Real numeric array of time points onto which you want to resample the data.
<i>method</i>	Method to use during resampling. Can be one of the following: <ul style="list-style-type: none">• 'interp1q' — Uses the MATLAB function interp1q.• — To use the MATLAB function interp1, specify one of the following methods:<ul style="list-style-type: none">▪ '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, `resample` uses the default time vector as described above.

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

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

Examples

Simulating and Resampling Data

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

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

- 2 Resample the data.

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

Resampling Data for Ensemble Runs

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

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

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

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

resample (SimData)

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

3 Interpolate the time steps.

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

4 View the time steps in the SimData object arrays.

```
newSimDataObj(1).Time  
simDataObj(1).Time
```

See Also

sbioensemblerun, sbioensemblestats, sbiosimulate, SimData
object

MATLAB functions `interp1`, `interp1q`

Purpose Delete all model objects from root object

Syntax `reset(sbioroot)`

Description `reset(sbioroot)` deletes all SimBiology model objects contained by the root object. This call is equivalent to `sbioreset`.

The root object contains a list of model objects, available units, unit prefixes, and kinetic laws.

To add a kinetic law to the user-defined library, use the `sbioaddtolibrary` function. To add a unit to the user-defined library, use the function `sbioregisterunit`. To add a unit prefix to the user-defined library, use the function `sbioregisterunitprefix`.

Examples **1** Query `sbioroot`, which has two model objects.

```
sbioroot
```

```
SimBiology Root Contains:
```

```
Models: 2
Builtin Abstract Kinetic Laws: 3
User Abstract Kinetic Laws: 1
Builtin Units: 54
User Units: 0
Builtin Unit Prefixes: 13
User Unit Prefixes: 0
```

2 Call `reset`.

```
sbioroot
```

```
SimBiology Root Contains:
```

```
Models: 0
Builtin Abstract Kinetic Laws: 3
User Abstract Kinetic Laws: 1
```

reset (root)

Builtin Units:	54
User Units:	0
Builtin Unit Prefixes:	13
User Unit Prefixes:	0

See Also

`sbioaddtolibrary`, `sbiohelp`, `sbioregisterunit`,
`sbioregisterunitprefix`, `sbioreset`, `sbioroot`

Purpose Remove contents from variant object

Syntax `rmcontent(variantObj, contents)`
`rmcontent(variantObj, idx)`

Arguments

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

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

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

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

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:	Value:
1	species	A	InitialAmount	5
2	species	B	InitialAmount	10
3	species	C	InitialAmount	15

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

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

```
SimBiology Variant - v1 (inactive)
```

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

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

```
rmcontent(variantObj, {'species','A', 'InitialAmount', 5});  
% Display variant object  
variantObj  
SimBiology Variant - v1 (inactive)
```

ContentIndex:	Type:	Name:	Property:	Value:
1	species	C	InitialAmount	15

See Also

addvariant, rmcontent, sbiovariant

rmproduct (reaction)

Purpose Remove species object from reaction object products

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

Arguments

<i>reactionObj</i>	Reaction object.
<i>SpeciesName</i>	Name for a model object. Enter a species name or a cell array of species names.
<i>speciesObj</i>	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 is returned.

Examples

Example 1

This example shows 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

<i>reactionObj</i>	Reaction object.
<i>SpeciesName</i>	Name for a species object. Enter a species name or a cell array of species names.
<i>speciesObj</i>	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

This example shows how to remove a reactant that was added to a reaction by mistake. You can remove the species object using the species name.

```
modelObj = sbiomodel('cell');  
reactionObj = addreaction(modelObj, 'Phosphocreatine + ADP + Pi -> 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

`delete`, `rmproduct`

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 built in (`BuiltinLibrary`), and the other contains components that are user defined (`UserdefinedLibrary`).

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

See “Property Summary” on page 4-153 for links to root object property reference pages.

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

Constructor Summary	<code>sbioroot</code>	Return SimBiology root object
----------------------------	-----------------------	-------------------------------

Method Summary	<code>copyobj</code> (any object)	Copy SimBiology object and its children
	<code>get</code> (any object)	Get object properties
	<code>reset</code> (root)	Delete all model objects from root object
	<code>set</code> (any object)	Set object properties

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 object, KineticLaw 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. For a description of the types of SimBiology rules, see `RuleType`.

See “Property Summary” on page 4-154 for links to rule property reference pages.

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

Constructor Summary

<code>addrule (model)</code>	Create rule object and add to model object
------------------------------	--

Method Summary

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

Property Summary

<code>Active</code>	Indicate object in use during simulation
<code>Annotation</code>	Store link to URL or file
<code>Name</code>	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 object, KineticLaw object, Model object, Parameter object, Reaction object, Root object, Species object

ScheduleDose object

Purpose Define drug dosing protocol

Description A ScheduleDose object defines a series of doses to the amount of a species during a simulation. The TargetName property defines the species that receives the dose.

Each dose can have a different amount, as defined by an amount array in the Amount property. Each dose can be given at specified times, as defined by a time array in the Time property. A rate array in the Rate property defines how fast each dose is given. At each time point in the time array, a dose is given with the corresponding amount and rate.

To use a dose object in a simulation, you must add the dose object to a model object and set the Active property of the dose object to true.

When there are multiple active ScheduleDdose objects on a model, and there are duplicate specifications for a property value, the simulation uses the last occurrence for the property value in the array of doses. You can find out which dose you applied last by looking at the indices of the dose objects stored on the model.

See the “Property Summary” on page 4-184 for links to species property reference pages. Properties define the characteristics of an object. Use the get command to list object properties and the set command to change their values at the command line. Use can graphically change object properties in the graphical user interface

Constructor Summary

sbiodose	Construct dose object
----------	-----------------------

Method Summary

Methods for variant objects

copyobj (any object)	Copy SimBiology object and its children
get (any object)	Get object properties
set (any object)	Set object properties

Property Summary

Properties for variant objects

Active	Indicate object in use during simulation
Amount	Amount of dose
AmountUnits	Dose amount units
Annotation	Store link to URL or file
DurationParameterName	Specify parameter with length of time
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rate	Amount of dose
RateUnits	Units for dose rate
Tag	Specify label for SimBiology object
TargetName	Species receiving dose
Time	Simulation time steps or schedule dose times
TimeUnits	Show stop time units for simulation
Type	Display top-level SimBiology object type
UserData	Specify data to associate with object

See Also

Model object, RepeatDose object, sbiodose, sbiosimulate

select (SimData)

Purpose Select data from SimData object

Syntax
`[t,x, names] = select(simDataObj, Query)`
`[Out] = select(simDataObj, Query, 'Format', 'FormatValue')`

Arguments Output Arguments

<i>t</i>	An n-by-1 vector of time points.
<i>x</i>	An n-by-m data array. <i>t</i> and <i>names</i> label the rows and columns of <i>x</i> respectively.
<i>names</i>	An m-by-1 cell array of names.
<i>Out</i>	Data returned in the format specified in 'FormatValue', shown in "Input Arguments" on page 4-158. Depending on the specified 'FormatValue', <i>Out</i> contains one of the following: <ul style="list-style-type: none">• Structure array• SimData object• Time series object• Combined time series object from an 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 `sbiiselect`. You can use any of the metadata fields available in the cells of the `DataInfo` property of a `SimData` object in a query. These include 'Type', 'Name', 'Units', 'Compartment' (species only), or 'Reaction' (parameter only).

FormatValue Choose a format from the following table.

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

select (SimData)

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 4-158.

Examples

This example shows how to extract data of interest from your simulation data with the `select` method.

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

```
sbioloadproject gprotein_norules m1
```

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

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

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

selectbyname (SimData)

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 the format as specified in '*FormatValue*', shown in "Input Arguments" on page 4-162. Depending on the specified '*FormatValue*', *Out* contains one of the following:

- Structure array
- SimData object
- Time series object
- Combined time series object from an 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 `sbiiselect`. You can use any of the metadata fields available in the cells of the `DataInfo` property of a `SimData` object. These include 'Type', 'Name', 'Units', 'Compartment' (species only), or 'Reaction' (parameter only).

FormatValue Choose a format from the following table.

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

selectbyname (SimData)

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 <code>simDataObj</code> .
'tslumped'	Specifies the format that lets you return data in time series objects, combining data from each SimData object into a single time series.

Description

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

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

`Out = selectbyname(simDataObj, NameValue, 'Format', Format)` returns the data in the specified format. Valid formats are listed in “Input Arguments” on page 4-162.

Examples

```
% Get data for the species 'glucose' from the simdata array sdarray.
[t x n] = selectbyname(sdarray,'glucose');

% Get data for multiple states and return the results in a struct array.
s = selectbyname(sdarray,{'RexGFP';'nuc.GFP';'cytosol.GFP'},...
    'Format','struct');
```

See Also

`getdata`, `sbioselect`, `sbiosimulate`

Purpose Set object properties

Syntax
`set(Obj, 'PropertyName', PropertyValue)`
`set(Obj, 'PropertyName1', PropertyValue1, 'PropertyName2',
PropertyValue2...)`

Arguments

Obj Abstract kinetic law, compartment, configuration set, event, kinetic law, model, parameter, PKCompartment, PKData, PKModelDesign, PKModelMap, reaction, rule, SimData, species, or variant object.

'*PropertyName*' Name of the property to set.

PropertyValue Specify the value to set. Property values depend on the property being set. See the reference page for an object property for values that can be specified.

Description

`set(Obj, 'PropertyName', PropertyValue)` sets the property '*PropertyName*' of the object *Obj*, to *PropertyValue*.

`set(Obj, 'PropertyName1', PropertyValue1, 'PropertyName2', PropertyValue2...)` sets the properties '*PropertyName1*' and '*PropertyName2*' to *PropertyValue1* and *PropertyValue2* respectively, and so on in sequence. You can specify multiple *PropertyName, PropertyValue* pairs.

When you want to change the name of a compartment, parameter, or species object, use the `rename` method instead of `set`. The `rename` method allows you to change the name and update the expressions in which these components are used.

Examples

1 Create a model object.

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

2 Add parameter object.

set (any object)

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

- 3 Set the ConstantValue property of the parameter object to false and verify.

MATLAB returns 1 for true and 0 for false.

```
set (parameterObj, 'ConstantValue', false);  
get(parameterObj, 'ConstantValue')
```

MATLAB returns

```
ans =
```

```
0
```

See Also

get , rename, setactiveconfigset

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]
```

setactiveconfigset (model)

```
SolverType: 'sundials'  
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 Specify specific parameters in kinetic law object

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

Arguments

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

Description Configure ParameterVariableNames in the kinetic law object.

`setparameter(kineticlawObj, 'ParameterVariablesValue', 'ParameterVariableNamesValue')` configures the ParameterVariableNames property of the kinetic law object (*kineticlawObj*). ParameterVariableValue corresponds to one of the strings in *kineticlawObj* ParameterVariables property. The corresponding element in the *kineticlawObj*ParameterVariableNames property is configured to ParameterVariableNamesValue. For example, if ParameterVariables is {'Vm', 'Km'} and ParameterVariablesValue is specified as Vm, then the first element of the ParameterVariableNames cell array is configured to ParameterVariableNamesValue.

Examples

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

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

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

setparameter (kineticlaw)

```
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

Purpose

Specify species in kinetic law object

Syntax

```
setspecies(kineticlawObj, 'SpeciesVariablesValue',  
           'SpeciesVariableNamesValue')
```

Arguments

<i>SpeciesVariablesValue</i>	Specify the species variable in the kinetic law object.
<i>SpeciesVariableNamesValue</i>	Specify the species name with which to configure the species variable in the kinetic law object. Determines the species in the ReactionRate equation.

Description

setspecies configures the kinetic law object SpeciesVariableNames property.

```
setspecies(kineticlawObj, 'SpeciesVariablesValue',  
           'SpeciesVariableNamesValue')
```

 configures the SpeciesVariableNames property of the kinetic law object, kineticlawObj. SpeciesVariablesValue corresponds to one of the strings in the SpeciesVariables property of kineticlawObj. The 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.

Examples

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

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

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

setspecies (kineticlaw)

- 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

Purpose

Simulation data storage

Description

The SimBiology SimData object contains simulation data. The output from the `sbiosimulate` function, is stored in the SimData object which holds time and state data as well as metadata, such as the types and names for the logged states or the configuration set used during simulation.

You can also store data from multiple simulation runs as an array of SimData objects. Thus, the output of `sbioensemblerun` is an array of SimData objects. You can use any SimData method on an array of SimData objects.

You can access the time, data, and metadata stored in the SimData object through the properties in “Property Summary” on page 4-174. Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line.

Methods you can use to query the SimData object are listed in “Method Summary” on page 4-173.

Constructor Summary

<code>sbioensemblerun</code>	Multiple stochastic ensemble runs of SimBiology model
<code>sbiosimulate</code>	Simulate model object

Method Summary

<code>delete (any object)</code>	Delete SimBiology object
<code>display (any object)</code>	Display summary of SimBiology object
<code>get (any object)</code>	Get object properties
<code>getdata (SimData)</code>	Get data from SimData object array

SimData object

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
set (any object)	Set object properties

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	Simulation time steps or schedule dose times
TimeUnits	Show stop time units for simulation
UserData	Specify data to associate with object

Examples

Return simulation results to a SimData object and plot the results.

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

Get simulation data at specific time points using the resample method.

```
% Load 'radiodecay' and set the initial amount of species 'x'.
sbioloadproject('radiodecay', 'm1');
x = sbioselect(m1, 'Type', 'species', 'Name', 'x');
x.InitialAmount = 100;
% Change the solver type to a stochastic solver.
cs = m1.getconfigset;
cs.SolverType = 'ssa';
% Simulate the model.
simDataObj = sbiosimulate(m1);
% This result could be misinterpreted as containing fractional mole
sbioplot(simDataObj);
title('Simulation Results Before Resampling');
%Resample the data using the zero-order hold method to obtain the c
%number of molecules at intermediate time steps.
newsimDataObj = resample(simDataObj, linspace(0, 10, 1e4), 'zoh');
sbioplot(newsimDataObj);
title('Simulation Results After Resampling');
```

Initialize a simulation using results from a previous simulation.

```
% Load 'radiodecay'.
sbioloadproject('radiodecay', 'm1');
m1.Species
simDataObj = sbiosimulate(m1);
% Use the Data property to get the states at the final time point.
% Data 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.
finaldata = simDataObj.Data(end,:);
% Use the DataInfo property to get names of states.
info = simDataObj.DataInfo;
```

SimData object

```
% Loop through the states (species) and set their initial amounts.
numSpecies = length(info);
for c = 1:numSpecies
    compObj = sbioselect(m1,'type','compartment','Name',info{c}.CompartmentName);
    speciesObj = sbioselect(compObj,'type','species','Name',info{c}.Name);
    speciesObj.InitialAmount = finaldata(c);
end
% Verify species initial amounts.
m1.Species
```

See Also

Model object, Parameter object, Reaction object, Root 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. The process of adding the reaction to the model 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 click **Species** to open the **Species** pane.

See “Property Summary” on page 4-178 for links to species property reference pages. Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

<code>addspecies (compartment)</code>	Create species object and add to compartment object
---------------------------------------	---

Method Summary

Methods for species objects

<code>copyobj (any object)</code>	Copy SimBiology object and its children
<code>delete (any object)</code>	Delete SimBiology object
<code>display (any object)</code>	Display summary of SimBiology object
<code>get (any object)</code>	Get object properties

Species object

rename (compartment,
parameter, species)

Rename object and update
expressions

set (any object)

Set object properties

Property Summary

Properties for species objects

Annotation

Store link to URL or file

BoundaryCondition

Indicate species boundary
condition

ConstantAmount

Specify variable or constant
species amount

InitialAmount

Species initial amount

InitialAmountUnits

Species initial amount units

Name

Specify name of object

Notes

HTML text describing SimBiology
object

Parent

Indicate parent object

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

Purpose

Hold information about user-defined unit

Description

The SimBiology unit object holds information about user-defined units. To create a unit, create the unit object and add the unit to the library using the `sbioaddtolibrary` function.

Use the unit object property `Composition` to specify the composition of your units. See “Property Summary” on page 4-179 for links to unit object property reference pages.

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

Constructor Summary

<code>sbiounit</code>	Create user-defined unit
-----------------------	--------------------------

Method Summary

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

Property Summary

<code>Annotation</code>	Store link to URL or file
<code>Composition</code>	Unit composition
<code>Multiplier</code>	Relationship between defined unit and base unit
<code>Name</code>	Specify name of object

Unit 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

Purpose

Hold information about user-defined unit prefix

Description

The SimBiology unit prefix object holds information about user-defined unit prefixes. To create a unit prefix, create the unit prefix object and add the unit prefix to the library using the `sbioaddtolibrary` function.

Use the unit prefix object property `Exponent`, to specify the exponent of your unit prefix. See “Property Summary” on page 4-181 for links to unit prefix object property reference pages.

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

Constructor Summary

<code>sbiounitprefix</code>	Create user-defined unit prefix
-----------------------------	---------------------------------

Method Summary

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

Property Summary

<code>Annotation</code>	Store link to URL or file
<code>Exponent</code>	Exponent value of unit prefix
<code>Name</code>	Specify name of object
<code>Notes</code>	HTML text describing SimBiology object
<code>Parent</code>	Indicate parent object

UnitPrefix 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

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 4-184 for links to species property reference pages. Properties define the characteristics of an object. Use the `get` and `set` commands to list object properties and change

Variant object

their values at the command line. You can graphically change object properties in the graphical user interface.

Constructor Summary

<code>sbiovariant</code>	Construct variant object
--------------------------	--------------------------

Method Summary

Methods for variant objects

<code>addcontent (variant)</code>	Append content to variant object
<code>commit (variant)</code>	Commit variant contents to model
<code>copyobj (any object)</code>	Copy SimBiology object and its children
<code>delete (any object)</code>	Delete SimBiology object
<code>display (any object)</code>	Display summary of SimBiology object
<code>get (any object)</code>	Get object properties
<code>rmcontent (variant)</code>	Remove contents from variant object
<code>set (any object)</code>	Set object properties
<code>verify (model, variant)</code>	Validate and verify SimBiology model

Property Summary

Properties for variant objects

<code>Active</code>	Indicate object in use during simulation
<code>Annotation</code>	Store link to URL or file
<code>Content</code>	Contents of variant object
<code>Name</code>	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, Model object, Parameter object, Species object
sbiosimulate

verify (model, variant)

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 **Errors and Warnings** pane.

Examples

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

See Also `sbiolasterror`, `sbiolastwarning`

Property Reference

Abstract Kinetic Law (p. 5-3)	Properties for abstract kinetic law objects
Compartments (p. 5-4)	Properties for compartment objects
Configuration Sets (p. 5-5)	Properties for configuration set objects
Events (p. 5-6)	Properties for event objects
Kinetic Laws (p. 5-7)	Properties for kinetic law objects
Models (p. 5-8)	Properties for model objects
NMFileDef (p. 5-9)	Properties for NMFileDef objects
Parameters (p. 5-10)	Properties for parameter objects
PKCompartment (p. 5-11)	Properties for PKCompartment objects
PKData (p. 5-12)	Properties for PKData objects
PKModelDesign (p. 5-13)	Properties for PKModelDesign objects
PKModelMap (p. 5-14)	Properties for PKModelMap objects
Reactions (p. 5-15)	Properties for reaction objects
RepeatDose (p. 5-16)	Properties for RepeatDose objects
Root (p. 5-17)	Properties for the root object
Rules (p. 5-18)	Properties for rule objects
ScheduleDose (p. 5-19)	Properties for ScheduleDose objects
SimData (p. 5-20)	Properties for SimData objects

Species (p. 5-21)

Unit (p. 5-21)

Unit Prefix (p. 5-22)

Variant (p. 5-22)

Using Object Properties (p. 5-24)

Properties for species objects

Properties for unit objects

Properties for unit objects

Properties for variant objects

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 kinetic law definition
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
StartTime	Start time for simulation or initial dose time
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 kinetic law definition
Parent	Indicate parent object
SpeciesVariableNames	Cell array of species 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

NMFileDef

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

PKCompartment

DosingType	Drug dosing type in compartment
EliminationType	Drug elimination type from compartment
HasResponseVariable	Compartment drug concentration reported
Name	Specify name of object

PKData

CovariateLabels	Identify covariate columns in data set
DataSet	Dataset object containing imported data
DependentVarLabel	Identify dependent variable column in data set
DependentVarUnits	Response units in PKData object
DoseLabel	Dose column in data set
DoseUnits	Dose units in PKData object
GroupID	Integer identifying each group in data set
GroupLabel	Identify group column in data set
GroupNames	Unique values from GroupLabel in data set
IndependentVarLabel	Identify independent variable column in data set
IndependentVarUnits	Time units in PKData object
RateLabel	Rate of infusion column in data set
RateUnits	Units for dose rate

PKModelDesign

PKCompartments

Hold compartments in PK model

PKModelMap

Dosed	Dosed object name
DosingType	Drug dosing type in compartment
Estimated	Names of parameters to estimate
Observed	Measured response object name
ZeroOrderDurationParameter	Zero order dose absorption duration

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

RepeatDose

Active	Indicate object in use during simulation
Amount	Amount of dose
AmountUnits	Dose amount units
Annotation	Store link to URL or file
DurationParameterName	Specify parameter with length of time
Interval	Amount of dose
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rate	Amount of dose
RateUnits	Units for dose rate
RepeatCount	Dose repetitions
StartTime	Start time for simulation or initial dose time
Tag	Specify label for SimBiology object
TargetName	Species receiving dose
TimeUnits	Show stop time units for simulation
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

ScheduleDose

Active	Indicate object in use during simulation
Amount	Amount of dose
AmountUnits	Dose amount units
Annotation	Store link to URL or file
DurationParameterName	Specify parameter with length of time
Name	Specify name of object
Notes	HTML text describing SimBiology object
Parent	Indicate parent object
Rate	Amount of dose
RateUnits	Units for dose rate
Tag	Specify label for SimBiology object
TargetName	Species receiving dose
Time	Simulation time steps or schedule dose times
TimeUnits	Show stop time units for simulation
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	Simulation time steps or schedule dose times
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. 5-24)	Use either MATLAB functions or object dot notation to enter or change property values.
Retrieving Property Values (p. 5-24)	Use either MATLAB functions or object dot notation to get property values.
Help for Objects, Methods, and Properties (p. 5-25)	Use the command <code>sbiohelp</code> 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.

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

Properties — Alphabetical List

AbsoluteTolerance

Purpose Specify largest allowable absolute error

Description The AbsoluteTolerance property specifies the largest allowable absolute error at any step in simulation. It is a property of SolverOptions object. SolverOptions is a property of the configset object. AbsoluteTolerance is available for the ode solvers ('sundials', '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:

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

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. For generated pharmacokinetic models default is 1e-15.
Access	Read/write

Examples

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

Characteristics

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

Examples

1 Create a model object.

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


- 2 Add a reaction object and verify that the Active property setting is 'true' or 1.

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

MATLAB returns:

```
ans =  
  
1
```

- 3 Set the Active property to 'false' and verify.

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

MATLAB returns:

```
ans =  
  
0
```

See Also

addconfigset, addreaction, addrule, Event object, Reaction object, RepeatDose object, Rule object, ScheduleDose object, Variant object,

Amount

Purpose Amount of dose

Description Amount is a property of a RepeatDose or ScheduleDose object. It defines an increase in the amount of a SimBiology species or an increase in the value of a SimBiology parameter that receives a dose.

A RepeatDose object defines a series of doses. Each dose is the same amount, as defined by the Amount property, and given at equally spaced times, as defined by the Interval property. The number of injections in the series, excluding the initial injection, is defined by the RepeatCount property, and the Rate property defines how fast each dose is given.

A ScheduleDose object defines a series of doses. Each dose can have a different amount, as defined by an amount array in the Amount property, and given at specified times, as defined by a time array in the Time property. A rate array in the Rate property defines how fast each dose is given. At each time point in the time array, a dose is given with the corresponding amount and rate.

Characteristics

Applies to	Object: RepeatDose, ScheduleDose
Data type	double (RepeatDose) or double array (ScheduleDose)
Data values	Default value is 0 (RepeatDose) or [] (ScheduleDose)
Access	Read/write

See Also ScheduleDose object and RepeatDose object

Purpose Dose amount units

Description AmountUnits is a property of a RepeatDose or ScheduleDose object. This property defines units for the Amount property.

If the TargetName property defines a species, then AmountUnits for a dose must be a chemical amount (for example, milligram, mole, or molecule), not a concentration. To get a list of the defined units in the library, use the sbioshowunits function. To add a user-defined unit to the list, see sbioaddtolibrary.

Characteristics

Applies to	Objects: RepeatDose, ScheduleDose
Data type	string
Data values	Units from library with dimensions of amount. Default = "" (empty)
Access	Read/write

Examples

See Also ScheduleDose object and RepeatDose object

Annotation

Purpose Store link to URL or file

Description The Annotation property stores the URL or file name linking to information about a model.

Characteristics

Applies to	SimBiology objects: abstract kinetic law, configuration set, compartment, event, kinetic law, model, parameter, reaction, RepeatDose, rule, ScheduleDose, species, or unit
Data type	char string, URL
Data values	Character string with a directory path and filename or a URL
Access	Read/write

Examples

1 Create a model object.

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

2 Set the annotation for a 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, RepeatDose object, ScheduleDose object

Purpose

Indicate species boundary condition

Description

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

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

More Information

Consider the following two use cases of boundary conditions:

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

Formation of the chaperone-receptor complex,

```
Hsp90_complex + GR_cyt -> Hsp90_complex:GR_cyt
```

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

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

BoundaryCondition

For dex,

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

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

```
ddex/dt = 0.001
```

which is specified in the SimBiology software as

```
dex = 0.001
```

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

Examples

- 1 Create a model object.

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

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

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

MATLAB returns:

```
ans =  
  
0
```

- 3 Set the boundary condition to 'true' and verify.

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

MATLAB returns:

```
ans =  
  
1
```

References

Pratt, W.B., Galigniana, M.D., Morishima, Y., Murphy, P.J. (2004), Role of molecular chaperones in steroid receptor action, *Essays Biochem*, 40:41-58.

See Also

addrule, addspecies, ConstantAmount, InitialAmount

BuiltInKineticLaws

Purpose Contain built-in kinetic laws

Note BuiltInKineticLaws has been removed and produces an error. Use BuiltInLibrary instead.

Description BuiltInKineticLaws is a SimBiology root object property showing all abstract kinetic laws that are shipped with the SimBiology software. Use the command `sbiowhos -builtin -kineticlaw` to see the list of built-in kinetic laws. You can use built-in kinetic laws when you use the command `addkineticlaw` to create a kinetic law object for a reaction object. Refer to the kinetic law by name when you create the kinetic law object, for example:

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

You cannot add, modify, or delete BuiltInKineticLaws.

See “Kinetic Law Definition” on page 6-61 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

Purpose Library of built-in components

Description `BuiltInLibrary` is a SimBiology root object property containing all built-in components namely, unit, unit-prefixes, and 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 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 “Kinetic Law Definition” on page 6-61 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` has been removed and produces an error. 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.

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`

Purpose Contain built-in units

Note BuiltInUnits has been removed and produces an error. Use BuiltInLibrary instead.

Description BuiltInUnits is a SimBiology root object property showing all units that are shipped with SimBiology. You can specify units for species amounts and parameter values to do dimensional analysis and unit conversion during simulation. The valid units are either built-in or user-defined. You can display the built-in units either by using the command `sbiowhos`, or by accessing the root object.

You cannot add, modify, or delete BuiltInUnits.

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.

Note 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 the capacity having a negative value.

Characteristics

Applies to	Object: compartment
Data type	double
Data values	Positive real number. The default value is 1.
Access	Read/write

Examples

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

- 1 Create a model object named my_model.

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

- 2 Add the compartment object named nucleus with a capacity of 0.5.

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

See Also

addcompartment, addspecies, CapacityUnits, ConstantCapacity

Purpose Compartment capacity units

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

Characteristics

Applies to	Object: compartment
Data type	char string
Data values	Units from library with dimensions of length, area, or volume. Default = '' (empty).
Access	Read/write

Examples

1 Create a model object named my_model.

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

2 Add a compartment object named cytoplasm with a capacity of 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
```

CapacityUnits

See Also

InitialAmount, sbioaddtolibrary, sbioconvertunits,
sbioshowunits

Purpose Array of compartments in model or compartment

Description `Compartments` shows you a read-only array of SimBiology compartment objects in the model object and the compartment object. In the model object, the `Compartments` property indicates all the compartments in a `Model` object as a flat list. In the compartment object, the `Compartments` property indicates other compartments that are referenced within the compartment. The two instances of `Compartments` are illustrated in “Examples” on page 6-21.

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

Characteristics

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

Examples

1 Create a model object named `modelObj`.

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

2 Add two compartments to the model object.

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

3 Add a compartment to one of the compartment objects.

```
compartmentObj3 = addcompartment(compartmentObj2, 'matrix');
```

4 Display the `Compartments` property in the model object.

```
get(modelObj, 'Compartments')
```

```
SimBiology Compartment Array
```

Compartments

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	Dimension of species name in expression
DimensionalAnalysis	Perform dimensional analysis on model
Type	Display top-level SimBiology object type
UnitConversion	Perform unit conversion

Characteristics

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

Examples

1 Retrieve the configset object of modelObj.

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

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

CompileOptions

```
optionsObj = get(configsetObj, 'CompileOptions');
```

Compile Settings:

```
UnitConversion:      false  
DimensionalAnalysis: true
```

See Also `get`, `set`

Purpose Unit composition

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

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

Characteristics

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

Examples

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

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

```
unitObj = sbiunit('secondconstant', '1/molarity*second', 1);
```

- 2 Query the Composition property.

```
get(unitObj, 'Composition')
```

```
ans =
```

```
1/molarity*second
```

- 3 Change the Composition property.

Composition

```
set(unitObj, 'Composition', 'liter/mole*second')  
  
ans =  
  
liter/mole*second
```

4 Add the unit to the user-defined library.

```
sbioaddtolibrary(unitObj);
```

See Also

get, Multiplier, Offset, sbiounit, set

Purpose Specify variable or constant species amount

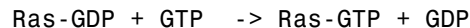
Description The ConstantAmount property indicates whether the quantity of the species object can vary during the simulation. ConstantAmount can be either true or false. If ConstantAmount is true, the quantity of the species cannot vary during the simulation. By default, ConstantAmount is false and the quantity of the species can vary during the simulation. If ConstantAmount is false, the quantity of the species can be determined by reactions and rules.

The property ConstantAmount is for species objects; the property ConstantValue is for parameter objects.

More Information

The following is an example of modeling species as constant amounts:

Modeling the role of nucleotides (GTP, ATP, cAMP) and cofactors (Ca⁺⁺, NAD⁺, coenzyme A). Consider the role of GTP in the activation of Ras by receptor tyrosine kinases.



Model GTP and GDP with constant amount set to true. In addition, you can set the BoundaryCondition of these species to true, thus making them *boundary species*.

Characteristics

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

Examples

1 Create a model object named my_model.

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

ConstantAmount

- 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 the 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

Examples

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

- 1 Create a model object named comp_model.

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

- 2 Add the compartment object named nucleus with a capacity of 0.5.

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

- 3 Display the ConstantCapacity property.

```
get(compartmentObj, 'ConstantCapacity')
```

```
ans =
```

```
1
```

See Also

addcompartment, ConstantAmount, ConstantValue

ConstantValue

Purpose Specify variable or constant parameter value

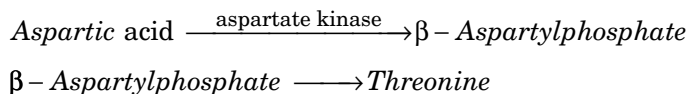
Description The ConstantValue property indicates whether the value of a parameter can change during a simulation. Enter either `true` (value is constant) or `false` (value can change).

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:



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`.

$$\text{k_aspartate_kinase} - (1/\text{threonine})$$

Characteristics

Applies to	Object: parameter
Data type	boolean

Data values	true or false. The default value is 'true'.
Access	Read/write

Examples

- 1 Create a model object.

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

- 2 Add a 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

Content

Purpose Contents of variant object

Description The Content property contains the data for the variant object. Content is a cell array with the structure {'Type', 'Name', 'PropertyName', 'PropertyValue'}. You can store values for species InitialAmount, parameter Value, and compartment Capacity, in a variant object.

For more information about variants, see Variant object.

Characteristics

Applies to	Object: variant
Data type	cell array
Data values	Default value is [] (empty).
Access	Read/write

Examples

1 Create a model containing three species in one compartment.

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

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

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

```
SimBiology Variant - v1 (inactive)
```

ContentIndex:	Type:	Name:	Property:	Value:
1	species	A	InitialAmount	5
2	species	B	InitialAmount	10

3 Append data to the Content property.

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

```
SimBiology Variant - v1 (inactive)
```

ContentIndex:	Type:	Name:	Property:	Value:
1	species	A	InitialAmount	5
2	species	B	InitialAmount	10
3	species	C	InitialAmount	15

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

`addcontent`, `rmcontent`, `sbiovariant`

CovariateLabels

Purpose Identify covariate columns in data set

Description CovariateLabels is a property of the PKData object. It specifies the column in DataSet that contains that contain the covariate data.

Characteristics

Applies to	Object: PKData
Data type	char string or cell array of strings
Data values	Column headers from imported data set
Access	Read/write

See Also and in the SimBiology User's Guide, PKData object

Purpose Store simulation data

Description The Data property contains the simulation data stored in the SimData object.

This property contains all data logged during a simulation, including species amounts, parameter values, and sensitivities. The property is an $m \times n$ array, where m is the number of time steps in the simulation and n is the number of quantities logged. The rows of the array are labeled by the time points in the Time property, and the columns are labeled by the metadata in the DataInfo property.

Characteristics

Applies to	Object: SimData
Data type	double
Data values	Default value is [] (empty).
Access	Read-only

See Also DataInfo, ModelName

DataCount

Purpose Numbers of species, parameters, sensitivities

Description The DataCount property shows how many species, parameters, and sensitivities are logged in a SimData object. It is a MATLAB structure with the fields Species, Parameter, and Sensitivity. The information in this property is redundant with the DataInfo property and is there to give you a convenient means to access the information.

Characteristics

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

See Also StopTime, StopTimeType

Purpose Metadata labels for simulation data

Description The DataInfo property contains the metadata that label the columns of the SimData object array. It is an $n \times 1$ cell array of structures. The i th cell contains metadata labeling the i th column of the SimData object array.

The possible types of structures are as follows.

Type	Fields
Species	Type: species Name: Compartment: Units:
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

DataInfo

Type	Fields
	Units: <code>the sensitivity input, for species or parameters, respectively></code>

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 that label the columns of the data matrix in the Data property. The property contains an nx1 array of strings. The software provides this information for your convenience.

Characteristics

Applies to	Object: SimData
Data type	string array
Data values	Default value is 0x1 cell array.
Access	Read-only

See Also StopTime, StopTimeType

DataSet

Purpose Dataset object containing imported data

Description DataSet is a property of the PKData object. It contains the imported data set. The PKData object constructor (PKData) assigns the specified data set to its DataSet property during construction.

Characteristics

Applies to	Object: PKData
Data type	dataset object
Data values	Variable containing dataset object
Access	Read-only

See Also in the SimBiology User's Guide, PKData object

Purpose Dimension of species name in expression

Description The `DefaultSpeciesDimension` property specifies how SimBiology interprets species names in expressions (namely reaction rate, rule, or event expressions). The valid property values are `substance` or `concentration`. If you specify `InitialAmountUnits`, SimBiology interprets species names appearing in expressions as concentration or substance amount according to the units specified, regardless of the value in `DefaultSpeciesDimension`. Thus, if `DefaultSpeciesDimension` is `concentration` and you specify species units as `molecule`, SimBiology interprets species names in expressions as `substance`. This interpretation applies even when `DimensionalAnalysis` is off.

You can find `DefaultSpeciesDimension` in the `CompileOptions` property.

When you set `DefaultSpeciesDimension` to `substance`, if you do not specify units, SimBiology interprets species names appearing in expressions as substance amounts, and does not scale by compartment capacity. To include a species concentration in an expression, divide by the appropriate compartment capacity in the expression. To specify compartment capacity in an expression enter the compartment name.

When you set `DefaultSpeciesDimension` to `concentration`, SimBiology interprets species names appearing in expressions as concentrations, and scales by compartment capacity in the expressions. To include a species amount in an expression, multiply by the species name by the appropriate compartment name in the expression.

See “Evaluation of Reaction Rate” in the SimBiology User’s Guide for information on dimensional analysis for reaction rates.

Characteristics

Applies to	Object: <code>CompileOptions</code> (in <code>configset</code> object)
Data type	<code>char</code> string

DefaultSpeciesDimension

Data values	concentration or substance. Default value is concentration.
Access	Read/write

See Also

CompileOptions, DimensionalAnalysis, get, getconfigset, sbiosimulate, set

Purpose Identify dependent variable column in data set

Description `DependentVarLabel` is a property of the `PKData` object. It specifies the column in `DataSet` that contains the dependent variable (for example, measured response). The column must contain numeric values, and cannot contain `Inf` or `-Inf`.

Characteristics

Applies to	Objects: <code>PKData</code>
Data type	<code>char string</code>
Data values	Column header from imported data set
Access	Read/write

See Also in the SimBiology User's Guide, `PKData` object

DependentVarUnits

Purpose Response units in PKData object

Description The `DependentVarUnits` property indicates the units for the column containing the dependent variable (response) in the imported data. If unit conversion is on, plot results in the SimBiology desktop show the units specified in `DependentVarUnits`.

To get a list of units, use the `sbioshowunits` function.

Characteristics

Applies to	Object: PKData
Data type	string
Data values	Units from units library. Default is '' (empty).
Access	Read/write

See Also `DependentVarLabel`, PKData Object

Purpose

Perform dimensional analysis on model

Description

The `DimensionalAnalysis` property specifies whether to perform dimensional analysis on the model before simulation. It is a property of the `CompileOptions` object. `CompileOptions` holds the model's compile time options and is the object property of the `configset` object. When `DimensionalAnalysis` is set to `true`, the SimBiology software checks whether the physical quantities of the units involved in reactions and rules, match and are applicable.

For example, consider a reaction $a + b \rightarrow c$. Using mass action kinetics, the reaction rate is defined as $a \cdot b \cdot k$, 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 $1 / (M \cdot \text{second})$. If you specify k with another equivalent unit definition, for example, $1 / [(\text{moles/liter}) \cdot \text{second}]$, `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: <code>CompileOptions</code> (in <code>configset</code> object)
Data type	<code>boolean</code>

DimensionalAnalysis

Data values	true or false. Default value is true.
Access	Read/write

Examples

This 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:      sundials
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

get, getconfigset, sbiosimulate, set

Dosed

Purpose Dosed object name

Description Dosed is a property of the PKModelMap object. It specifies the name of an object that is receiving an input, such as a drug in a compartment or a ligand. Specify the name of a species, a compartment, or a parameter (scoped to a model).

Characteristics

Applies to	Objects: PKModelMap
Data type	char string or cell array of strings
Data values	Name of an object, or empty
Access	Read/write

See Also in the SimBiology User's Guide, Estimated, Observed, PKModelMap object

Purpose Dose column in data set

Description DoseLabel is a property of the PKData object. DoseLabel specifies the column that contains that contains the dosing information, in DataSet. The column must contain positive values, and cannot contain Inf or Inf.

Characteristics

Applies to	Object: PKData
Data type	string or array of strings
Data values	Column headers from imported data set
Access	Read/write

See Also PKData object, sbionmimport, sbionmfiledef, in the SimBiology documentation

DoseUnits

Purpose Dose units in PKData object

Description The `DoseUnits` property indicates the units for dose values in the PKData object. Dose units must have dimensions of amount or mass. The length of `DoseUnits` must be the same as `DoseLabel`. For example, if the `DoseLabel` property defines two columns containing dosing information, `DoseUnits` must also define units for both columns. If unit conversion is on, dose and rate units must be consistent with each other (that is in terms of amount or mass) and must be consistent with the species object that is being dosed.

To get a list of units, use the `sbioshowunits` function.

Characteristics

Applies to	Object: PKData
Data type	string or array of strings
Data values	Units from units library. Default is '' (empty).
Access	Read/write

See Also `DoseLabel`, PKData Object

Purpose Drug dosing type in compartment

Description DosingType is a property of the PKCompartment and PKModelMap objects. It specifies the type of dosing of a drug in a compartment. You can only dose one compartment in the model at any given time. For a description of the types of dosing supported, the model components created for each type of dosing, and the parameters to estimate, see in the SimBiology User's Guide.

Characteristics

Applies to	Objects: PKCompartment, PKModelMap
Data type	char string
Data values	'', 'Bolus', 'Infusion', 'ZeroOrder', 'FirstOrder'
Access	Read/write

See Also EliminationType, PKCompartment object, PKModelMap object

DurationParameterName

Purpose Specify parameter with length of time

Description DurationParameterName is a property of a RepeatDose or a ScheduleDose object that identifies a parameter scoped to a model. The parameter specifies the length of time it takes to administer a dose. The Amount property specifies the amount of the dose. Since the rate of dose is calculated from the amount and duration, you cannot specify the rate. Therefore, set the Rate property to zero.

Characteristics

Applies to	Objects: RepeatDose, ScheduleDose
Data type	char string
Data values	Any char string, except reserved words and characters
Access	Read/write

See Also RepeatDose object, ScheduleDose object

Purpose Drug elimination type from compartment

Description EliminationType is a property of the PKCompartment object. It specifies the type of elimination of adrug from a compartment. For a description of the types of elimination supported, the model components created for each type of elimination, and the parameters to estimate, see in the SimBiology User's Guide.

Characteristics

Applies to	Object: PKCompartment
Data type	char string
Data values	'Linear', 'Linear-Clearance', 'Enzymatic', and ''
Access	Read/write

See Also addCompartment, DosingType, PKCompartment object

ErrorTolerance

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 (τ) such that the relative change in the propensity function for each reaction is less than the user-specified error tolerance.

A propensity function describes the probability that the reaction will occur in the next smallest time interval, given the conditions and constraints.

If the error tolerance is too large, there may not be a solution to the problem and that could lead to an error. If the error tolerance is small, the solver will take more steps than when the error tolerance is large leading to longer simulation times. The error tolerance should be adjusted depending upon the problem, but a good value for the error tolerance is between 1 % to 5 %.

Characteristics

Applies to	Object: SolverOptions
Data type	double
Data values	>0, <1. The default is $3e-2$.
Access	Read/write

Examples

This example shows how to change ErrorTolerance settings.

- 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

Estimated

Purpose Names of parameters to estimate

Description Estimated is a property of the PKModelMap object. It specifies the name of the objects to estimate. Specify the name of a species, compartment, or parameter.

Characteristics

Applies to	Objects: PKModelMap
Data type	char string or cell array of strings
Data values	Name of objects
Access	Read/write

See Also in the SimBiology User's Guide, Dosed, Observed, PKModelMap object

Purpose Event expression

Description Property of the event object that defines what occurs when the event is triggered. Specify a cell array of strings.

EventFcns can be any MATLAB assignment or expression that defines what is executed when the event is triggered. All EventFcn expressions are assignments of the form '*objectname* = *expression*', where *objectname* is the name of a valid SimBiology object.

For more information about how SimBiology handles events, see “How Events Are Evaluated” in the SimBiology User’s Guide documentation. For examples of event functions, see “Specifying Event Functions” in the SimBiology User’s Guide documentation.

Characteristics

Applies to	Object: event
Data type	Cell array of strings
Data values	EventFcn strings '' (empty)
Access	Read/write

Examples

1 Create a model 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 = 0pA', '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 “Changing Model Component Values Using Events” in the SimBiology User’s Guide documentation for more information.

Add an event to a Model object with the `addevent` method and remove an event with the `delete` method. See `Event` object for more information.

You can view event object properties with the `get` command and modify the properties with the `set` command.

Characteristics

Applies to	Object: model
Data type	Array of event objects
Data values	Event object. The default is [] (empty).
Access	Read-only

Examples

1 Create a model object, and then 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

EventFcns, Event object, Model object, 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	<code>double</code>
Data values	Real number. Default is 0.
Access	Read/write

Examples

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

1 Create a unit prefix.

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

2 Add the unit prefix to the user-defined library.

```
sbioaddtolibrary(unitprefixObj1);
```

3 Query the `Exponent` property.

```
get(unitprefixObj1, 'Exponent')
```

```
ans =
```

```
15
```

See Also

`get`, `sbioaddtolibrary`, `sbiounitprefix`, `set`, `UnitPrefix` object

Purpose

Expression to determine reaction rate equation

Description

The `Expression` property indicates the mathematical expression that is used to determine the `ReactionRate` property of the reaction object. `Expression` is a reaction rate expression assigned by the kinetic law definition used by the reaction. The kinetic law being used is indicated by the property `KineticLawName`. You can configure `Expression` for user-defined kinetic laws, but not for built-in kinetic laws. `Expression` is read only for kinetic law objects.

Kinetic Law Definition

The *kinetic law definition* provides a mechanism for applying a specific rate law to multiple reactions. It acts as a mapping template for the reaction rate. The kinetic law is defined by a mathematical expression, (defined in the property `Expression`), and includes 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 a kinetic law definition, the `ReactionRate` property of the reaction object shows the result of a mapping from the kinetic law definition. To determine `ReactionRate`, the species variables and parameter variables that participate in the reaction rate should be mapped in the kinetic law for the reaction. In this case, SimBiology software determines the `ReactionRate` by using the `Expression` property of the abstract kinetic law object, and by mapping `SpeciesVariableNames` to `SpeciesVariables` and `ParameterVariableNames` to `ParameterVariables`.

For example, the kinetic law definition Henri-Michaelis-Menten has the `Expression` $V_m * S / (K_m + S)$, where V_m and K_m 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 Henri-Michaelis-Menten kinetic law to a reaction $A \rightarrow B$ with V_a mapping to V_m , A mapping to S , and K_a mapping to K_m , the rate equation for the reaction becomes $V_a \cdot A / (K_a + A)$.

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

$$r = k \prod_{i=1}^{n_r} [S_i]^{m_i}$$

where $[S_i]$ is the concentration of the i th reactant, m_i is the stoichiometric coefficient of $[S_i]$, n_r is the number of reactants, and k is the mass action reaction rate constant.

SimBiology software contains some built-in kinetic laws. You can also define your own kinetic laws. To find the list of available kinetic laws, use the `sbiowhos -kineticlaw` command (`sbiowhos`). You can create a kinetic law definition with the function `sbioabstractkineticlaw` and add it to the library using `sbioaddtolibrary`.

Characteristics

Applies to	Objects: abstract kinetic law, kinetic law
Data type	char string
Data values	Defined by kinetic law definition
Access	Read-only in kinetic law object. Read/write in user-defined 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 (V_m and K_m) 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 V_m_d , K_m_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:

Expression

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

Example 2

Example with Mass Action kinetics.

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

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

- 2 Define a kinetic law for the reaction object.

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

MATLAB returns:

```
ans =  
  
MassAction
```

- 3 Assign the rate constant for the reaction.

```
set (kineticlawObj, 'ParameterVariableNames', 'k');  
  
get (reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =  
  
k*a*b
```

See Also

KineticLawName, Parameters, ParameterVariableNames, ParameterVariables, ReactionRate, sbioaddtolibrary, sbiowhos, SpeciesVariables, SpeciesVariableNames

Purpose Integer identifying each group in data set

Description GroupID is a property of the PKData object. It is an array of the same length as the DataSet property containing an integer to identify each group. PKData sets this property during construction of the PKData object.

Characteristics

Applies to	Object: PKData
Data type	double
Data values	Index value for each group
Access	Read-only

See Also in the SimBiology User's Guide, PKData object

GroupLabel

Purpose Identify group column in data set

Description GroupLabel is a property of the PKData object. It specifies the column in DataSet that contains the group identification labels.

Characteristics

Applies to	Object: PKData
Data type	char string
Data values	Column header string from imported data set
Access	Read/write

See Also in the SimBiology User's Guide, PKData object, GroupNames

Purpose Unique values from `GroupLabel` in data set

Description `GroupNames` is a property of the `PKData` object. It contains unique values from the data column specified by the `GroupLabel` property. `PKData` sets this property during construction of the `PKData` object.

Characteristics

Applies to	Object: <code>PKData</code>
Data type	<code>char</code> string or cell array of strings
Data values	Unique values in <code>GroupLabel</code>
Access	Read-only

See Also in the SimBiology User's Guide, `PKData` object, `GroupLabel`

HasResponseVariable

Purpose Compartment drug concentration reported

Description HasResponseVariable is a property of the PKCompartment object. It is a logical indicating if the drug concentration in this compartment is reported.

Characteristics

Applies to Objects: PKCompartment

Data type logical

Data values 1 (true) or 0 (false).

Access Read/write

See Also addCompartment, DosingType, EliminationType, PKCompartment object

Purpose Identify independent variable column in data set

Description IndependentVarLabel is a property of the PKData object. It specifies the column in DataSet that contains the independent variable (for example, time).

The column must contain positive values, and cannot contain, NaN, Inf or -Inf.

Characteristics

Applies to	Object: PKData
Data type	char string
Data values	Column header from imported data set

Access	Read/write
--------	------------

See Also in the SimBiology User's Guide, PKData object

IndependentVarUnits

Purpose Time units in PKData object

Description The IndependentVarUnits property indicates the units for the column containing the independent variable (time) in the PKData object. If unit conversion is on, plot results in the SimBiology desktop show the units specified in IndependentVarUnits.

To get a list of units, use the sbioshowunits function.

Characteristics

Applies to	Object: PKData
Data type	string
Data values	Time units. Default is '' (empty).
Access	Read/write

See Also DependentVarLabel, PKData Object

Purpose Species initial amount

Description The `InitialAmount` property indicates the initial quantity of the SimBiology species object. `InitialAmount` is the quantity of the species before the simulation starts.

Characteristics

Applies to	Object: species
Data type	double
Data values	Positive real number. Default value is 0.
Access	Read/write

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

1 Create a model object named `my_model`.

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

2 Add the species object named `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`

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 built-in units. To get a list of the defined units, use the `sbiowunits` function. If `InitialAmountUnits` changes from one unit definition to another, `InitialAmount` does not automatically convert to the new units. The `sbiconvertunits` 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 $\text{amount}/\text{meter}^2$ 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 is '' (empty).
Access	Read/write

Examples

1 Create a model object named `my_model`.

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

2 Add a species object named `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, sbioconvertunits, sbioregisterunit, sbioshowunits

Interval

Purpose Amount of dose

Description Interval is a property of a RepeatDose object. This property defines the equally spaced times between repeated doses.

Characteristics

Applies to	Object: RepeatDose
Data type	double
Data values	Positive real number. Default value is 0
Access	Read/Write

See Also ScheduleDose object and RepeatDose object

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 you update the reaction, the ReactionRate property automatically updates only for mass action kinetics. For all other kinetics, you must set the SpeciesVariableNames property of the kinetic law object.

See “Evaluation of Reaction Rate” in the SimBiology User’s Guide for information on dimensional analysis for reaction rates.

Characteristics

Applies to	Object: reaction
Data type	Kinetic law object
Data values	Kinetic law object. Default is [] (empty).
Access	Read-only

Examples

Example with Henri-Michaelis-Menten kinetics

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

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

- 2 Define a kinetic law for the reaction object.

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

- 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

KineticLawName, Parameters, ParameterVariableNames, ReactionRate, SpeciesVariableNames

Purpose Name of kinetic law applied to reaction

Description The `KineticLawName` property of the kinetic law object indicates the name of the kinetic law definition applied to the reaction. `KineticLawName` can be any valid name from the built-in or user-defined kinetic law library. See “Kinetic Law Definition” on page 6-61 for more information.

You can find the `KineticLawName` list in the kinetic law library by using the command `sbiowhos -kineticlaw (sbiowhos)`. You can create a kinetic law definition with the function `sbioabstractkineticlaw` and add it to the library using `sbioaddtolibrary`.

Characteristics

Applies to	Object: <code>kineticlaw</code>
Data type	<code>char string</code>
Data values	<code>char string</code> specified by kinetic law definition
Access	Read-only

Examples

- 1 Create a model object, add a reaction object, and define a kinetic law for the reaction object.

```
modelObj = sbiomodel ('my_model');  
reactionObj = addreaction (modelObj, 'a + b -> c + d');  
kineticlawObj = addkineticlaw(reactionObj, 'Henri-Michaelis-Menten');
```

- 2 Verify the `KineticLawName` of `kineticlawObj`.

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

MATLAB returns:

```
ans =  
  
Henri-Michaelis-Menten
```

KineticLawName

See Also

Expression, Parameters, ParameterVariableNames,
ParameterVariables, ReactionRate, sbioaddtolibrary, sbiowhos,
SpeciesVariables, SpeciesVariableNames

Purpose Specify recorded simulation output frequency

Description The LogDecimation property defines how often the simulation data is recorded as output. It is a property of the SolverOptions object. SolverOptions is a property of the configset object. LogDecimation is available for ssa, expltau, and inmpltau solvers.

Use LogDecimation to specify how frequently you want to record the output of the simulation. For example, if the LogDecimation is set to 1, for the command (t,x) = sbiosimulate(modelObj), at each simulation step the time will be logged in t and the quantity of each logged species will be logged as a row in x. If LogDecimation is 10, then every 10th simulation step will be logged in t and x.

Characteristics

Applies to	Object: SolverOptions
Data type	int
Data values	>0. Default is 1.
Access	Read/write

Examples This example shows how to change LogDecimation settings.

- 1 Retrieve the configset object from the modelObj, and change the SolverType to expltau.

```
modelObj = sbiomodel('cell');  
configsetObj = getconfigset(modelObj);  
set(configsetObj, 'SolverType', 'expltau')
```

- 2 Change the LogDecimation to 10.

```
set(configsetObj.SolverOptions, 'LogDecimation', 10);  
get(configsetObj.SolverOptions, 'LogDecimation')
```

```
ans =
```

LogDecimation

10

See Also

ErrorTolerance, RandomState

Purpose Specify nonlinear solver maximum iterations in implicit tau

Description The `MaxIterations` property specifies the maximum number of iterations for the nonlinear solver in `impltau`. It is a property of the `SolverOptions` object. `SolverOptions` is a property of the `configset` object.

The implicit tau solver in SimBiology software internally uses a nonlinear solver to solve a set of algebraic nonlinear equations at every simulation step. Starting with an initial guess at the solution, the nonlinear solver iteratively tries to find the solution to the algebraic equations. The closer the initial guess is to the solution, the fewer the iterations the nonlinear solver will take before it finds a solution. `MaxIterations` specifies the maximum number of iterations the nonlinear solver should take before it issues a “failed to converge” error. If you get this error during simulation, try increasing `MaxIterations`. The default value of `MaxIterations` is 15.

Characteristics

Applies to	Object: <code>SolverOptions</code>
Data type	<code>int</code>
Data values	>0. Default is 15.
Access	Read/write

Examples

This 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);
```

MaxIterations

```
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 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 or empty
Data values	Default value is [] (empty). When the SolverType is <code>sundials</code> , [] is equivalent to setting MaxStep to infinity. For all other solvers, [] is equivalent to setting the MaxStep to $0.1 * \text{StopTime}$.
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 '' (empty).
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 `sbiupdate` 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`, `sbiupdate`

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	Nonzero real number. Default value is 1.
Access	Read/write

Examples

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

- 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`, `get`, `Offset`, `sbiounit`, `set`

Purpose

Specify name of object

Description

The Name property identifies a SimBiology object. Compartments, species, parameters, and model objects can be referenced by other objects using the Name property, therefore Name must be unique for these objects. However, species names need only be unique within each compartment. Parameter names must be unique within a model (if at the model level), or within each kinetic law (if at the kinetic law level). This means that you can have nonunique species names if the species are in different compartments, and nonunique parameter names if the parameters are in different kinetic laws or at different levels. Note that having nonunique parameter names can cause the model to have shadowed parameters and that may not be best modeling practice. For more information on levels of parameters, see “Definition of Parameter Scope” in the SimBiology User’s Guide documentation.

Use the function `sbioselect` to find an object with the same Name property value.

In addition, note the following constraints and reserved characters for the Name property in objects:

- Model names cannot be empty.
- Parameter names cannot be empty, or have the name `time`.
- If you have a parameter, a species, or compartment name that is not a valid MATLAB variable name, when you write an event function, an event trigger, a reaction, reaction rate equation, or a rule you must enclose that name in brackets. For example, enclose `[DNA polymerase+]` in brackets. In addition, if you have the same species in multiple compartments you must qualify the species with the compartment name, for example, `nucleus.[DNA polymerase+]`, `[nuclear complex].[DNA polymerase+]`.
- Species and compartment names cannot be empty, and note the following reserved words, characters, and constraints:

Name

- The literal words `null` and `time`. Note that you can specify species names with these words contained within the name. For example, `nullaminoacids` or `nullnucleotides`.
- The characters `->`, `< >`, `[`, and `]`.

For more information on valid MATLAB variable names, see `genvarname` and `isvarname`.

Characteristics

Applies to	Objects: abstract kinetic law, configuration set, compartment, event, kinetic law, model, parameter, reaction, RepeatDose, rule, ScheduleDose, species, unit, or variant
Data type	char string
Data values	Any char string except reserved words and characters
Access	Read/write

Examples

- 1 Create a model object named `my_model`.

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

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

```
reactionObj = addreaction(modelObj, '[Aspartic acid] -> [beta-Aspartyl-P04]')
```

MATLAB returns:

```
SimBiology Reaction Array
```

```
Index:   Reaction:  
1       [Aspartic acid] -> [beta-Aspartyl-P04]
```

- 3 Set the reaction Name and verify.

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

MATLAB returns:

```
ans =
```

```
Aspartate kinase reaction
```

See Also

addcompartment, addkineticlaw, addmodel, addparameter,
addreaction, addrule, addspecies, RepeatDose object, sbiomodel,
sbionunit, sbionunitprefix, ScheduleDose object

Normalization

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: <code>SensitivityAnalysisOptions</code>
Data type	enum
Data values	'None', 'Half', 'Full'. Default is 'None'.
Access	Read/write

See Also `ParameterInputFactors`, `SensitivityAnalysis`, `SensitivityAnalysisOptions`, `SpeciesInputFactors`

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, RepeatDose, rule, ScheduleDose, species, unit, or unit prefix
Data type	char string
Data values	Any char string
Access	Read/write

Examples

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`, `RepeatDose` object, `sbiomodel`, `sbiounit`, `sbiounitprefix`, `ScheduleDose` object

Observed

Purpose Measured response object name

Description Observed is a property of the PKModelMap object. It specifies the name of an object that represents the measured response (the response variable). Specify the name of a species, compartment, or parameter.

Characteristics

Applies to	Object: PKModelMap
Data type	char string or cell array of strings
Data values	Names of objects
Access	Read/write

See Also in the SimBiology User's Guide, Dosed, Estimated, PKModelMap object

Purpose Unit composition modifier

Description

Note The `Offset` property is currently not supported.

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 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 =
```

Offset

32

See Also

Composition, get, Multiplier, sbioaddtolibrary, sbioshowunits, sbiounit, set

Purpose Owing compartment

Description Owner shows you the SimBiology compartment object that owns the compartment object. In the compartment object, the Owner property shows you whether the compartment resides within another compartment. The Compartments property indicates whether other compartments reside within the compartment. You can add a compartment object using the method addcompartment.

Characteristics

Applies to	Object: compartment
Data type	char string
Data values	Name of compartment object. Default is [].
Access	Read-only

Examples

- 1 Create a model object named modelObj.

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

- 2 Add two compartments to the model object.

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

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

```
compartmentObj3 = addcompartment(compartmentObj2, 'matrix');
```

- 4 Display the Owner property in the compartment objects.

```
get(compartmentObj3, 'Owner')
```

The result shows you the owning compartment and its components:

```
SimBiology Compartment - mitochondrion
```

Owner

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

5 Change the owning compartment.

```
set(compartmentObj3, 'Owner', compartmentObj1)
```

See Also

Compartments, Parent

Purpose Specify parameter input factors for sensitivity analysis

Description `ParameterInputFactors` is a property of the `SensitivityAnalysisOptions` object. `SensitivityAnalysisOptions` is a property of the configuration set object. Use `ParameterInputFactors` to specify the parameters with respect to which you want to compute the sensitivities of the species states in your model. When you simulate a model with `SensitivityAnalysis` enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species specified in `StatesToLog`. For a description of the output, see the `SensitivityAnalysisOptions` property description.

Characteristics

Applies to	Object: <code>SensitivityAnalysisOptions</code>
Data type	Parameter object or array of parameter objects
Data values	Parameter object array. Default is [] (empty).
Access	Read/write

Examples

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

- 1 Import the radio decay model from the SimBiology demos.

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

- 2 Retrieve the configuration set object from `modelObj`.

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

- 3 Add a parameter to the `ParameterInputFactors` property and display. Use the `sbioselect` function to retrieve the parameter object from the model.

ParameterInputFactors

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

SimBiology Parameter Array

Index:	Name:	Value:	ValueUnits:
1	c	0.5	1/second

See Also

[sbioselect](#), [SensitivityAnalysis](#), [SensitivityAnalysisOptions](#),
[SpeciesInputFactors](#)

Purpose Array of parameter objects

Description The `Parameters` property indicates the parameters in a `Model` or `KineticLaw` object. Read-only array of `Parameter` objects.

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: <code>model</code> , <code>kineticlaw</code>
Data type	Array of parameter objects
Data values	Parameter objects. Default value is <code>[]</code> (empty).
Access	Read-only

Examples

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

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

2 Define a kinetic law for the reaction object.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

3 Add a parameter and assign it to the kinetic law object (`kineticlawObj`);

```
parameterObj1 = addparameter (kineticlawObj, 'K1');
```

Parameters

```
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, get, sbioparameter, set

Purpose Cell array of reaction rate parameters

Description The `ParameterVariableNames` property shows the parameters used by the kinetic law object to determine the `ReactionRate` equation in the reaction object. Use `setParameter` to assign `ParameterVariableNames`. When you assign species to `ParameterVariableNames`, SimBiology software maps these parameter names to `ParameterVariables` in the kinetic law object.

If the reaction is using a kinetic law, the `ReactionRate` property of a reaction object shows the result of a mapping from an “Kinetic Law Definition” on page 6-61. The `ReactionRate` is determined by the kinetic law object `Expression` property by mapping `ParameterVariableNames` to `ParameterVariables` and `SpeciesVariableNames` to `SpeciesVariables`.

Characteristics

Applies to	Object: <code>kineticlaw</code>
Data type	Cell array of strings
Data values	Cell array of parameters
Access	Read/write

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

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

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

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

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

`reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

ParameterVariableNames

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

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

- 4** Verify that the parameter variables are correct.

```
get (kineticlawObj, 'ParameterVariableNames')
```

MATLAB returns:

```
ans =  
  
    'Va'    'Ka'
```

See Also

Expression, ParameterVariables, ReactionRate, setparameter, SpeciesVariables, SpeciesVariableNames

Purpose

Parameters in kinetic law definition

Description

The `ParameterVariables` property shows the parameter variables that are used in the `Expression` property of the abstract kinetic law object. Use this property to specify the parameters in the `ReactionRate` equation. Use the method `set` to assign `ParameterVariables` to a kinetic law definition. For more information, see “Kinetic Law Definition” on page 6-61.

Characteristics

Applies to	Objects: abstract kinetic law, kineticlaw
Data type	Cell array of strings
Data values	Specified by kinetic law definition
Access	Read/write in kinetic law definition. Read-only in kinetic law.

Examples

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

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

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

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

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

reactionObj `KineticLaw` property is configured to kineticlawObj.

- 3 The 'Henri-Michaelis-Menten' kinetic law has two parameter variables. To set these variables:

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

ParameterVariables

MATLAB returns:

```
ans =
```

```
    'Vm'    'Km'
```

See Also

Expression, ParameterVariableNames, ReactionRate, set, setparameter, SpeciesVariables, SpeciesVariableNames

Purpose Indicate parent object

Description The Parent property indicates the parent object for a SimBiology object (read-only). The Parent property indicates accessibility of the object. The object is accessible to the Parent object and other objects within the Parent object. The value of Parent depends on the type of object and how it was created. All models always have the SimBiology root as the Parent.

More Information

The following table shows you the different objects and the possible Parent value.

Object	Parent
abstract kinetic law	<ul style="list-style-type: none"> • [] (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)
RepeatDose	model object or [] (empty)
rule	model object or [] (empty)
ScheduleDose	model object or [] (empty)
species	compartment

Parent

Object	Parent
variant	model object or [] (empty)
unit and unit prefixes	<ul style="list-style-type: none">• [] (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, RepeatDose, rule, ScheduleDose, species, variant, unit, or unit prefix
Data type	Object
Data values	SimBiology component object or [] (empty)
Access	Read-only

See Also

addkineticlaw, addmodel, addparameter, addreaction, RepeatDose object, sbiomodel, ScheduleDose object

Purpose Hold compartments in PK model

Description PKCompartments is a property of the PKModelDesign object. It is used to specify the compartments in the PKModelDesign object. Each compartment is a PKCompartment object added using the addCompartment method.

Characteristics

Applies to Objects: PKModelDesign

Data type object

Data values PKCompartment object

Access Read-only

See Also in the SimBiology User's Guide, addCompartment, PKCompartment object, PKModelDesign object

Products

Purpose Array of reaction products

Description The Products property contains an array of `SimBiology.Species` objects.

Products is a 1-by-n species object array that indicates the species that are changed by the reaction. If the Reaction property is modified to use a different species, the Products property is updated accordingly.

You can add product species to the reaction with `addproduct` function. You can remove product species from the reaction with `rmproduct`. You can also update reaction products by setting the Reaction property with the function `set`.

Characteristics

Applies to	Object: reaction
Data type	Array of objects
Data values	Species objects. Default is [] (empty).
Access	Read-only

Examples

1 Create a model object.

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

2 Add reaction objects.

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

3 Verify the 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`, `addproduct`, `addspecies`, `rmproduct`

RandomState

Purpose Set random number generator

Description The `RandomState` property sets the random number generator for the stochastic solvers. It is a property of the `SolverOptions` object. `SolverOptions` is a property of the `configset` object.

SimBiology software uses a pseudorandom number generator. The sequence of numbers generated is determined by the state of the generator, which can be specified by the integer `RandomState`. If `RandomState` is set to integer J , the random number generator is initialized to its J^{th} state. The random number generator can generate all the floating-point numbers in the closed interval $[2^{(-53)}, 1 - 2^{(-53)}]$. Theoretically, it can generate over 2^{1492} values before repeating itself. But for a given state, the sequence of numbers generated will be the same. To change the sequence, change `RandomState`. SimBiology software resets the state at startup. The default value of `RandomState` is `[]`.

Characteristics

Applies to	Objects: <code>SolverOptions</code> for SSA, <code>expltau</code> , <code>impltau</code>
Data type	<code>int</code>
Data values	Default is <code>[]</code> (empty).
Access	Read/write

Examples

This 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

Rate

Purpose Amount of dose

Description Rate is a property of a RepeatDose or ScheduleDose object. This property defines how fast a dose is given.

Characteristics

Applies to	Objects: RepeatDose, ScheduleDose
Data type	double (RepeatDose) or double array (ScheduleDose)
Data values	Positive real number. Default value is 0 (RepeatDose) or [] (ScheduleDose)
Access	Read/Write

See Also ScheduleDose object and RepeatDose object

Purpose Units for dose rate

Description RateUnits is a property of a PKData, RepeatDose or ScheduleDose object.

- In RepeatDose or ScheduleDose objects, this property defines units for the Rate property.
- In PKData object, this property defines units for the RateLabel property.

Characteristics

Applies to	Object: RepeatDose, ScheduleDose, PKData
Data type	string
Data values	Units from library with dimensions of amount divided by time. You cannot use units of concentration divided by time. Default = "
Access	Read/write

See Also PKData object, ScheduleDose object, RepeatDose object, Rate, RateLabel

RateLabel

Purpose Rate of infusion column in data set

Description RateLabel is a property of the PKData object. It specifies the column in DataSet that contains the rate of infusion. This applies only when dosing type is infusion. The data set must contain the rate and not an infusion time. The values must be positive and the column cannot contain Inf or -Inf. 0 specifies an infinite rate (equivalent to a bolus dose), and NaN specifies no rate.

Characteristics

Applies to	Objects: PKData
Data type	char string
Data values	Column header string
Access	Read/write

See Also in the SimBiology User's Guide, PKData object, DosingType

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	Object: reaction
Data type	Species object or array of species objects
Data values	Species objects. Default is [] (empty).
Access	Read-only

Examples

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

Reactants

2 unnamed b 0

See Also

addreactant, addreaction, addspecies, 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 '' (empty).
Access	Read/write

Examples

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

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

- 2 Verify that the reaction property records the input.

```
get (reactionObj, 'Reaction')
```

MATLAB returns:

```
ans =  
  
a + b -> c + d
```

See Also `addreaction`, `sbioreaction`

ReactionRate

Purpose Reaction rate equation in reaction object

Description The `ReactionRate` property defines the reaction rate equation. You can define a `ReactionRate` with or without the `KineticLaw` property. `KineticLaw` defines the type of reaction rate. The `addkineticlaw` function configures the `ReactionRate` based on the `KineticLaw` and the species and parameters specified in the kinetic law object properties `SpeciesVariableNames` and `ParameterVariableNames`.

The reaction takes place in the reverse direction if the `Reversible` property is true. This is reflected in `ReactionRate`. The `ReactionRate` includes the forward and reverse rate if reversible.

You can specify `ReactionRate` without `KineticLaw`. Use the `set` function to specify the reaction rate equation. SimBiology software adds species variables while creating `reactionObj` using the `addreaction` method. You must add the parameter variables (to the `modelObj` in this case). See the example below.

After you specify the `ReactionRate` without `KineticLaw` and you later configure the `reactionObj` to use `KineticLaw`, the `ReactionRate` is unset until you specify `SpeciesVariableNames` and `ParameterVariableNames`.

See “Evaluation of Reaction Rate” in the SimBiology User’s Guide for information on dimensional analysis for reaction rates.

Characteristics

Applies to	Object: reaction
Data type	char string
Data values	Reaction rate string. Default is '' (empty).
Access	Read/write

Examples **Example 1**

Create a model, add a reaction, and assign the expression for the reaction rate equation.

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

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

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

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

reactionObj.KineticLaw property is configured to kineticlawObj.

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

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

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

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

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

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

MATLAB returns:

```
ans =
```

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

Example 2

Create a model, add a reaction, and specify ReactionRate without a kinetic law.

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

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

- 2 Specify ReactionRate and verify the assignment.

```
set (reactionObj, 'ReactionRate', 'k*a');  
get(reactionObj, 'ReactionRate')
```

MATLAB returns:

```
ans =
```

```
k*a
```

- 3 You cannot simulate the model until you add the parameter k to the modelObj.

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

SimBiology adds the parameter to the modelObj with default Value = 1.0 for the parameter.

See Also

addparameter, addreaction, Reversible, sbioparameter, sbioreaction

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	Object: model
Data type	Array of reaction objects
Data values	Reaction object
Access	Read-only

Examples

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

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

2 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 `addreaction`, `delete`, `sbioreaction`

RelativeTolerance

Purpose Specify allowable error relative to component

Description The `RelativeTolerance` property specifies the allowable error tolerance relative to the state vector at each simulation step. The state vector contains values for all the state variables, for example, species amounts for all the species.

`RelativeTolerance` is a property of the `SolverOptions` object. `SolverOptions` is a property of the `configset` object. `RelativeTolerance` is available for the ode solvers ('sundials', '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

Examples

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, 'RelativeTolerance', 1.0e-6);  
get(configsetObj.SolverOptions, 'RelativeTolerance')
```

```
ans =
```

```
1.0000e-006
```

See Also

AbsoluteTolerance

RepeatCount

Purpose Dose repetitions

Description RepeatCount is a property of a RepeatDose object. This property defines the number of doses after the initial dose in a repeat dose series.

Characteristics

Applies to	Object: RepeatDose
Data type	double
Data values	Positive real number. Default value is 0
Access	Read/Write

See Also ScheduleDose object and RepeatDose object

Purpose Specify whether reaction is reversible or irreversible

Description The `Reversible` property defines whether a reaction is reversible or irreversible. The rate of the reaction is defined by the `ReactionRate` property. For a reversible reaction, the reaction rate equation is the sum of the rate of the forward and reverse reactions. The type of reaction rate is defined by the `KineticLaw` property. If a reaction is changed from reversible to irreversible or vice versa after `KineticLaw` is assigned, the new `ReactionRate` is determined only if `Type` is `MassAction`. All other `Types` result in unchanged `ReactionRate`. For `MassAction`, the first parameter specified is assumed to be the rate of the forward reaction.

Characteristics

Applies to	Object: reaction
Data type	boolean
Data values	true, false. Default value is false.
Access	Read/write

Examples

Create a model, add a reaction, and assign the expression for the reaction rate equation.

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

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

- 2 Set the `Reversible` property for the `reactionObj` to true and verify this setting.

```
set (reactionObj, 'Reversible', true)  
get (reactionObj, 'Reversible')
```

MATLAB returns:

```
ans =
```

1

MATLAB returns 1 for true and 0 for false.

In the next steps the example illustrates how the reaction rate equation is assigned for reversible reactions.

- 3 Create a kinetic law object for the reaction object of the type 'MassAction'.

```
kineticlawObj = addkineticlaw(reactionObj, 'MassAction');
```

reactionObj KineticLaw property is configured to kineticlawObj.

- 4 The 'MassAction' kinetic law for reversible reactions has two parameter variables ('Forward Rate Parameter' and 'Reverse Rate Parameter') that you should set. The species variables for MassAction are automatically determined. To set the parameter variables, first create the parameter variables as parameter objects (parameterObj1, parameterObj2) named Kf and Kr and assign the object to kineticlawObj.

```
parameterObj1 = addparameter(kineticlawObj, 'Kf');  
parameterObj2 = addparameter(kineticlawObj, 'Kr');
```

- 5 Set the variable names for the kinetic law object.

```
set(kineticlawObj, 'ParameterVariableNames', {'Kf' 'Kr'});
```

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

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

MATLAB returns:

```
ans =
```

```
Kf*a*b - Kr*c*d
```

See Also

`addparameter`, `addreactant`, `addreaction`, `ParameterVariableNames`,
`ReactionRate`, `sbioreaction`

Rule

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

Examples

1 Create a model object, and 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`.

The types of rules in SimBiology are as follows:

- `initialAssignment` — Lets you specify the initial value of a parameter, species, or compartment capacity, as a function of other model component values in the model.
- `repeatedAssignment` — Lets you specify a value that holds at all times during simulation, and is a function of other model component values in the model.
- `algebraic` — Lets you specify mathematical constraints on one or more parameters, species, or compartments that must hold during a simulation.
- `rate` — Lets you specify the time derivative of a parameter value, species amount, or compartment capacity.

Constraints on Varying Species Using a Rate Rule

If the model has a species defined in concentration, being varied by a rate rule, and it is in a compartment with varying volume, you can only use `rate` or `initialAssignment` rules to vary the compartment volume.

Conversely, if you are varying a compartment's volume using a `repeatedAssignment` or `algebraic` rules, then you cannot vary a species (defined in concentration) within that compartment, with a rate rule.

The reason for these constraints is that, if a species is defined in concentration and it is in a compartment with varying volume, the time derivative of that species is a function of the compartment's rate of change. For compartments varied by rate rules, the solver has that information.

Note that if you specify the species in amounts there are no constraints.

Characteristics

Applies to	Object: rule
Data type	char string
Data values	'initialAssignment', 'repeatedAssignment' 'algebraic', 'rate'. Default value is 'initialAssignment'.
Access	Read/write

Examples

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

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

- 2 Add a rule that specifies the quantity of a species c. In the rule expression, k is the rate constant for a -> b.

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

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

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

MATLAB returns all the properties for the rule object.

```
Active: 1
Annotation: ''
Name: ''
```

RuleType

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

See Also

“Changing Model Component Values Using Rules” in the *SimBiology User’s Guide*, `addrule`, `delete`, `sbiorule`

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

Examples

1 Create a model object, and 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`

RunInfo

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 `sbioensemblerrun`.

Characteristics

Applies to	Object: SimData
Data type	struct
Data values	Default values are as follows:

```
ConfigSet: []  
SimulationDate: ''  
SimulationType: ''  
Variant: []
```

In practice, the `ConfigSet`, `SimulationDate`, and `SimulationType` fields are rarely empty, since they are populated after simulation.

Access	Read-only
--------	-----------

See Also StopTime, StopTimeType

Purpose Options for logged species

Description The RuntimeOptions property holds options for species that will be logged during the simulation run. The run-time options object can be accessed through this property.

The LogDecimation property of the configuration set object defines how often data is logged.

Property 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

Examples

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 get, set

SensitivityAnalysis

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 ('sundials', 'ode45', 'ode23', 'ode113', 'ode15s', 'ode23s', 'ode23t', and 'ode23tb').

See `SensitivityAnalysisOptions` for more information on setting up sensitivity analysis. See “Sensitivity Analysis” in the SimBiology User’s Guide documentation for a description of sensitivity analysis calculations.

Characteristics

Applies to	Object: <code>SolverOptions</code>
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

SensitivityAnalysisOptions

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 6-139.

When sensitivity analysis is enabled, the following command

```
[t,x, names] = sbiosimulate(modelObj)
```

returns `[t,x, names]`, where

- `t` is an n -by-1 vector, where n is the number of steps taken by the ode solver and `t` defines the time steps of the solver.
- `x` is an n -by- m matrix, where n is the number of steps taken by the ode solver and m is:

```
Number of states specified in StatesToLog +  
(Number of species specified in StatesToLog*Number of input factors)
```

A SimBiology state includes species and nonconstant parameters.

- `names` is the list of states logged and the list of sensitivities of the species specified in `StatesToLog` with respect to the input factors.

For an example of the output, see “Examples” on page 6-139.

You can add a number of configuration set objects with different `SensitivityAnalysisOptions` to the model object with the `addconfigset` method. Only one configuration set object in the model object can have the `Active` property set to `true` at any given time.

Property Summary

Normalization	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
Data type	Object
Data values	SensitivityAnalysisOptions properties as summarized in “Property Summary” on page 6-139.
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'));
```

SensitivityAnalysisOptions

```
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” on page 6-138 for more information.

```
[t,x,names] = sbiosimulate(modelObj);
```

- 7** Display the names.

```
names
```

```
names =
```

```
'x'  
'z'  
'd[x]/d[z]_0'
```



```
'd[z]/d[z]_0'  
'd[x]/d[c]'  
'd[z]/d[c]'
```

8 Display state values `x`.

```
x
```

The display follows the column order shown in `names` for the values in `x`. The rows correspond to `t`.

See Also

`addconfigset`, `getconfigset`

SolverOptions

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 “Property Summary” on page 6-142.

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 (sundials).
Access	Read-only

Examples

This example shows the changes in SolverOptions for various SolverType settings.

- 1 Retrieve the configset object from the modelObj.

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

- 2 Configure the SolverType to ode45.

```
set(configsetObj, 'SolverType', 'ode45');  
get(configsetObj, 'SolverOptions')
```

```
Solver Settings: (ode)
```

```
AbsoluteTolerance: 1.000000e-006  
RelativeTolerance: 1.000000e-003
```

- 3 Configure the SolverType to ssa.

```
set(configsetObj, 'SolverType', 'ssa');  
get(configsetObj, 'SolverOptions')
```

```
Solver Settings: (ssa)
```

```
LogDecimation: 1  
RandomState: []
```

- 4 Configure the SolverType to impltau.

SolverOptions

```
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`

Purpose Select solver type for simulation

Description The SolverType property lets you specify the solver to use for a simulation. For a discussion about solver types, see “Selecting a Solver” in the SimBiology User’s Guide documentation.

Changing the solver type changes the options (properties) specified in the SolverOptions property of the configset object. If you change any SolverOptions, these changes are persistent when you switch SolverType. For example, if you set the ErrorTolerance for the expltau solver and then change to impltau when you switch back to expltau, the ErrorTolerance will have the number you assigned.

Characteristics

Applies to	Object: configset
Data type	enum
Data values	'ssa', 'expltau', 'impltau', 'ode45', 'ode23', 'ode113', 'ode15s', 'ode23s', 'ode23t', 'ode23tb', 'sundials'. Default is 'sundials'.
Access	Read/write

Examples

1 Retrieve the configset object from the modelObj.

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

```
Configuration Settings - default (active)  
SolverType:          sundials  
StopTime:           10.000000
```

```
SolverOptions:  
AbsoluteTolerance:  1.000000e-006  
RelativeTolerance:  1.000000e-003
```

SolverType

```
SensitivityAnalysis:      false
RuntimeOptions:
  StatesToLog:           all
CompileOptions:
  UnitConversion:       false
  DimensionalAnalysis:  true
SensitivityAnalysisOptions:
  InputFactors:         0
  Outputs:              0
```

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
  SensitivityAnalysis:  false
RuntimeOptions:
  StatesToLog:         all
CompileOptions:
  UnitConversion:       false
  DimensionalAnalysis:  true
SensitivityAnalysisOptions:
  InputFactors:         0
  Outputs:              0
```

See Also `getConfigset, set`

Species

Purpose Array of species in compartment object

Description The `Species` property is a property of the compartment object and indicates all the species in a compartment object. `Species` is a read-only array of SimBiology species objects.

In the model object, `Species` contains a flat list of all the species that exist within all the compartments in the model. You should always access a species through its compartment rather than the model object. Use the format `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. `SensitivityAnalysisOptions` is a property of the configuration set object.

The SimBiology software calculates sensitivities with respect to the initial amounts of the species specified in this property. When you simulate a model with `SensitivityAnalysis` enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species specified in `StatesToLog`. For a description of the output, see the `SensitivityAnalysisOptions` property description.

Characteristics

Applies to	Object: <code>SensitivityAnalysisOptions</code>
Data type	Species object or array of species objects
Data values	Species object array. Default is [] (empty).
Access	Read/write

Examples This example shows how to set `SpeciesInputFactors` for sensitivity analysis.

- 1 Import the radio decay model from the SimBiology demos.

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

- 2 Retrieve the configuration set object from `modelObj`.

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

- 3 Add a species to the `SpeciesInputFactors` property and display. Use the `sbioselect` function to retrieve the species object from the model.

SpeciesInputFactors

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

SimBiology Species Array

Index:	Compartment:	Name:	InitialAmount:	InitialAmountUnits:
1	unnamed	z	0	molecule

See Also

ParameterInputFactors, sbioselect, SensitivityAnalysis,
SensitivityAnalysisOptions

Purpose Specify species outputs for sensitivity analysis

Description The `SpeciesOutputs` property allows you to specify the species for which you want to compute sensitivities. `SpeciesOutputs` is a property of the `SensitivityAnalysisOptions` object. `SensitivityAnalysisOptions` is a property of the configuration set object.

The SimBiology software calculates sensitivities with respect to the values of the parameters specified in `ParameterInputFactors` and the initial amounts of the species specified in `SpeciesInputFactors`. When you simulate a model with `SensitivityAnalysis` enabled in the active configuration set object, sensitivity analysis returns the computed sensitivities of the species specified in `SpeciesOutputs`. For a description of the output, see the `SensitivityAnalysisOptions` property description.

Characteristics

Applies to	Object: <code>SensitivityAnalysisOptions</code>
Data type	Species object or array of species objects
Data values	Species object array. Default is <code>[]</code> (empty).
Access	Read/write

Examples This example shows how to set `SpeciesOutputs` for sensitivity analysis.

- 1 Import the radio decay model from the SimBiology demos.

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

- 2 Retrieve the configuration set object from `modelObj`.

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

- 3 Add a species to the `SpeciesOutputs` property and display. Use the `sbioselect` function to retrieve the species object from the model.

SpeciesOutputs

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

SimBiology Species Array

Index:	Compartment:	Name:	InitialAmount:	InitialAmountUnits:
1	unnamed	z	0	molecule

See Also

ParameterInputFactors, sbioselect, SensitivityAnalysis, SensitivityAnalysisOptions, SpeciesInputFactors

Purpose Cell array of species in reaction rate equation

Description The `SpeciesVariableNames` property shows the species used by the kinetic law object to determine the `ReactionRate` equation in the reaction object. Use `setspecies` to assign `SpeciesVariableNames`. When you assign species to `SpeciesVariableNames`, SimBiology software maps these species names to `SpeciesVariables` in the kinetic law object.

The `ReactionRate` property of a reaction object shows the result of a mapping from kinetic law definition. The `ReactionRate` is determined by the kinetic law object `Expression` property by mapping `ParameterVariableNames` to `ParameterVariables` and `SpeciesVariableNames` to `SpeciesVariables`.

Characteristics

Applies to	Object: kinetic law
Data type	Cell array of strings
Data values	Cell array of species names
Access	Read/write

Examples

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

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

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

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

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

The `reactionObj` `KineticLaw` property is configured to `kineticlawObj`.

SpeciesVariableNames

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

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

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

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

MATLAB returns:

```
ans =
```

```
'a'
```

See Also

Expression, ParameterVariables, ParameterVariableNames, ReactionRate, setparameter, SpeciesVariables

Purpose Species in abstract kinetic law

Description This property shows species variables that are used in the `Expression` property of the kinetic law object to determine the `ReactionRate` equation in the reaction object. Use the MATLAB function `set` to assign `SpeciesVariables` to an abstract kinetic law. For more information, see abstract kinetic law.

Characteristics

Applies to	Objects: abstract kinetic law, kineticlaw
Data type	Cell array of strings
Data values	Defined by abstract kinetic law
Access	Read/write in abstract kinetic law. Read-only in kinetic law.

Examples

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

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

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

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

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

reactionObj `KineticLaw` property is configured to kineticlawObj.

- 3 View the species variable for 'Henri-Michaelis-Menten' kinetic law.

```
get(kineticlawObj, 'SpeciesVariables')
```

MATLAB returns:

SpeciesVariables

```
ans =
```

```
'S'
```

See Also

Expression, ParameterVariables, ParameterVariableNames, ReactionRate, set, setparameter, SpeciesVariableNames

Purpose Start time for simulation or initial dose time

Description StartTime is a property of a Configset or RepeatDose object.

Configset Object

For a simulation, the StartTime property defines a time to begin a simulation. A start time, other than zero, delays the start of the simulation.

RepeatDose Object

For a series of repeated doses, the StartTime property defines the amount of time that elapses before the first (initial) dose is given.

Characteristics

Applies to	Objects: Configset, RepeatDose
Data type	double (Configset)double (RepeatDose)
Data values	Positive real number less than the stop time (Configset). Default value is 0.Positive real number. Default value is 0 (RepeatDose)
Access	Read-write

See Also RepeatDose object, Configset object, StopTime, StopTimeType

StatesToLog

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

Examples

This example shows how to assign species to StatesToLog.

- 1 Create a model object by importing the file `oscillator.xml`.

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

- 2 Retrieve the first and second species in `modelObj`.

```
speciesObj1 = modelObj.Species(1);  
speciesObj2 = modelObj.Species(2);
```

- 3 Retrieve the `configsetObj` of `modelObj`.

```
configsetObj = getConfigset(modelObj);
```

- 4 Set the StatesToLog to record three species: two using the retrieved species objects and one using indexing and view the species in StatesToLog.

```
set (configsetObj.RuntimeOptions, 'StatesToLog', ...  
    [speciesObj1, speciesObj2, modelObj.Species(3)]);  
get(configsetObj.RuntimeOptions, 'StatesToLog')
```

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 $3\text{H} + \text{A} \rightarrow 2\text{C} + \text{F}$ 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 $2\text{H} + \text{A} \rightarrow 2\text{C} + 3\text{F}$.

The length of the **Stoichiometry** array is the sum of the **Reactants** array and the **Products** array. To remove a product or reactant from a reaction, use the **rmproduct** or **rmreactant** function. Add a product or reactant and set stoichiometry with methods **addproduct** and **addreactant**.

ODE solvers support **double** stoichiometry values such as 0.5. Stochastic solvers and dimensional analysis currently support only integers in **Stoichiometry**, therefore you must balance the reaction equation and specify integer values for these two cases.

$\text{A} \rightarrow \text{null}$ has a stoichiometry value of [- 1]. $\text{null} \rightarrow \text{B}$ 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 is [] (empty).
Access	Read/write

Stoichiometry

Examples

- 1 Create a reaction object.

```
modelObj = sbiomodel('cell');  
reactionObj = addreaction(modelObj, '2 a + 3 b -> d + 2 c');
```

- 2 Verify the Reaction and Stoichiometry properties for reactionObj.

```
get(reactionObj, 'Stoichiometry')
```

MATLAB returns:

```
ans =  
  
-2    -3     1     2
```

- 3 Set stoichiometry to [-1 -2 2 2].

```
set (reactionObj, 'Stoichiometry', [-1 -2 2 2]);  
get (reactionObj, 'Stoichiometry')
```

MATLAB returns:

```
ans =  
  
-1    -2     2     2
```

- 4 Note with get that the Reaction property updates automatically.

```
get (reactionObj, 'Reaction')
```

MATLAB returns:

```
ans =  
  
a + 2 b -> 2 d + 2 c
```

See Also

addproduct, addreactant, addreaction, Reaction, rmproduct, rmreactant

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

Examples

1 Retrieve the configset object from modelObj.

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

2 Configure the StopTime to 20.

```
set(configsetObj, 'StopTime', 20)  
get(configsetObj, 'StopTime')
```

```
ans =
```

```
20
```

See Also StopTimeType, TimeUnits

StopTimeType

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: <code>configset</code>
Data type	<code>enum</code>
Data values	<code>approxWallTime</code> , <code>numberOfLogs</code> , and <code>simulationTime</code>
Access	Read/write

Examples

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

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

2 Configure the `StopTimeType` to `approxWallTime`.

```
set(configsetObj, 'StopTimeType', 'approxWallTime');  
get(configsetObj, 'StopTimeType')  
  
ans =  
  
approxWallTime
```

See Also

set, StatesToLog, StopTime, TimeUnits

Purpose Specify label for SimBiology object

Description The Tag property specifies a label associated with a SimBiology object. Use this property to group objects and then use `sbioselect` to retrieve. For example, use the Tag property in reaction objects to group synthesis or degradation reactions. You can then retrieve all synthesis reactions using `sbioselect`. Similarly, for species objects you can enter and store classification information, for example, membrane protein, transcription factor, enzyme classifications, or whether a species is an independent variable. You can also enter the full form of the name of the species. This is useful when viewing the model in the Block Diagram Explorer. For example, the species object Name could be G6P for convenience, but in the Tag you should enter the full name, Glucose-6 phosphate. The graphical representation of the model in the Block Diagram Explorer (available in the SimBiology desktop: `simbiology`) 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, RepeatDose, rule, ScheduleDose, species
Data type	char string
Data values	Any char string
Access	Read/write

Examples

1 Create a model object.

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

2 Add a reaction object and set the Tag property to 'Synthesis Reaction'.

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


3 Verify the Tag assignment.

```
get (reactionObj, 'Tag');
```

MATLAB returns:

```
ans =
```

```
'Synthesis Reaction'
```

See Also

`addkineticlaw`, `addparameter`, `addreaction`, `addrule`, `addspecies`,
`RepeatDose object`, `sbioabstractkineticlaw`, `sbiomodel`, `sbiroot`

TargetName

Purpose Species receiving dose

Description TargetName is a property of a RepeatDose or ScheduleDose object. This property defines the SimBiology species receiving the dose. The dose amount increases the species amount at each time interval defined by a repeat dose or at each time point defined by a schedule dose.

The value of TargetName is the name of a species. If the model has more than one species with the same name, TargetName is defined as *compartmentName.speciesName*, where *compartmentName* is the name of the compartment containing the species.

Characteristics

Applies to	Objects: RepeatDose, ScheduleDose
Data type	string
Data values	Species name. Default value is "" (empty).
Access	Read/Write

See Also ScheduleDose object and RepeatDose object

Purpose Event trigger

Description A Trigger is a condition that must become true for an event to be executed. You can a combination of relational and logical operators to build a trigger expression. Trigger can be a string, an expression, or a function handle that when evaluated returns a value of true or false. Triggers can access species, parameters, and compartments.

A trigger can contain the keyword 'time', to define an event that occurs at a specific time during the simulation.

For more information about how the SimBiology software handles events, see “How Events Are Evaluated” in the SimBiology User’s Guide documentation. For examples of event functions, see “Specifying Event Triggers” in the SimBiology User’s Guide documentation.

Characteristics

Applies to	Object: event
SimBiology type	String, function handle
SimBiology values	Specify MATLAB expression as string. Default is '' (None).
Access	Read/write

Examples

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')
```

Trigger

See Also

Event object, EventFcms

Purpose Simulation time steps or schedule dose times

Description Time is a property of a SimData or ScheduleDose object.

SimData Object

For a simulation, the Time property records the time steps.

ScheduleDose Object

For a series of scheduled doses, the Time property defines the times to give a dose.

A ScheduleDose object defines a series of doses. Each dose can have a different amount, as defined by an amount array in the Amount property, and given at specified times, as defined by a time array in the Time property. A rate array in the Rate property defines how fast each dose is given. At each time point in the time array, a dose is given with the corresponding amount and rate.

Characteristics

Applies to	Object: SimData, ScheduleDose object
Data type	double (SimData), double array (ScheduleDose)
Data values	Vector of doubles (SimData)Array of positive real numbers. Default value is [] (ScheduleDose)
Access	Read-only

See Also ScheduleDose object, SimData object, StopTime, StopTimeType

TimeUnits

Purpose Show stop time units for simulation

Description The TimeUnits property specifies time units for the property Time.

Characteristics

Applies to	Objects: configset, RepeatDose, ScheduleDose
Data type	string
Data values	Default value is second.
Access	Read-only

See Also RepeatDose object, StopTime, StopTimeType, ScheduleDose object

Purpose Display top-level SimBiology object type

Description The Type property indicates a SimBiology object type. When you create a SimBiology object, the value of Type is automatically defined.

For example, when a Species object is created, the value of the Type property is automatically defined as 'species'.

Characteristics

Applies to	Objects: abstract kinetic law, configuration set, CompileOptions, kinetic law, model, parameter, reaction, RepeatDose, root, rule, ScheduleDose, species, RuntimeOptions, and SolverOptions
Data type	char string
Data values	abstract_kinetic_law, configset, compileoptions, kineticlaw, parameter, reaction, repeatdose, root, rule, runtimeoptions, sbiomodel, scheduledose, species, and solveroptions
Access	Read-only

See Also RepeatDose object, sbiomodel, sbioparameter, sbioreaction, sbioroot, sbiorule, sbiospecies, ScheduleDose object, setactiveconfigset

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`, the SimBiology software 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 $a + b \rightarrow c$. Using mass action kinetics the reaction rate is defined as $a \cdot b \cdot k$ 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`, the simulation uses the given object values.

Unit conversion involving temperature supports `Celsius` as the temperature unit. Avoid using mixed temperature units as you might get an error.

Characteristics

Applies to	Object: CompileOptions (in configset object)
Data type	boolean
Data values	true or false. Default value is false.
Access	Read/write

Examples

This 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:      sundials
StopTime:        10.000000
```

```
SolverOptions:
```

```
AbsoluteTolerance: 1.000000e-006
RelativeTolerance: 1.000000e-003
```

UnitConversion

```
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

get, getconfigset, sbiosimulate, 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, RepeatDose, rule, ScheduleDose, species, or unit
Data type	Any
Data values	Any. Default is empty.
Access	Read/write

See Also RepeatDose object, sbioabstractkineticlaw, sbiomodel, sbioparameter, sbioreaction, sbioroot, sbiorule, sbiospecies, sbiunit, sbiunitprefix, ScheduleDose object

UserDefinedKineticLaws

Purpose Contain user-defined kinetic laws

Note UserDefinedKineticLaws has been removed and produces an error. Use UserDefinedLibrary instead.

Description The UserDefinedKineticLaws property is a SimBiology root object property showing all user-defined kinetic law definitions. 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 a kinetic law definition 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 “Kinetic Law Definition” on page 6-61 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 AbstractKineticLaw object, `sbioaddtolibrary`, 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 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 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 “Kinetic Law Definition” on page 6-61 for a definition and more information.

Characteristics

Applies to	Object: root
Data type	object

UserDefinedLibrary

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

BuiltInLibrary, sbioaddtolibrary, sbioremovefromlibrary, sbioroot, sbiounit, sbiounitprefix

UserDefinedUnitPrefixes

Purpose Contain user-defined unit prefixes

Note UserDefinedUnitPrefixes has been removed and produces an error. Use UserDefinedLibrary instead.

Description The UserDefinedUnitPrefixes property is a SimBiology root object property showing all user-defined unit prefixes. You can specify units with prefixes for species amounts and parameter values to do dimensional analysis and unit conversion during simulation. The valid units and unit prefixes are either built in or user defined. Use the command `sbiowhos -userdefined -unit` to see the list of user-defined units.

You can add, modify, or delete UserDefinedUnitPrefixes. You can define a unit prefix with the command `sbioregisterunitprefix`, which enables you to create the unit and add it to the user-defined unit prefixes library, and also add it to the UserDefinedUnitPrefixes property of the root object.

Characteristics

Applies to	Object: root
Data type	char string
Data values	Valid unit prefixes
Access	Read/write

See Also `sbioaddtolibrary`, `UserDefinedLibrary`, `UnitPrefix` object

Purpose Contain user-defined units

Note UserDefinedUnits has been removed and produces an error. Use UserDefinedLibrary instead.

Description The UserDefinedUnits property is a SimBiology root object property showing all user-defined units. You can specify units for species amounts and parameter values to do dimensional analysis and unit conversion during simulation. The valid units are either built in or user defined. Use the command `sbiowhos -userdefined -unit` to see the list of user-defined units.

You can add, modify, or delete UserDefinedUnits. You can define a unit with the command `sbioregisterunit`, which enables you to create the unit and add it to the user-defined units library, and also add it to the UserDefinedUnits property of the root object.

Characteristics

Applies to	Object: root
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

Examples

Assign a parameter with a value to the model object.

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

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

- 2 Add a parameter to the model object (`modelObj`) with Value 0.5.

```
parameterObj1 = addparameter (modelObj, 'K1', 0.5)
```

MATLAB returns:

```
SimBiology Parameter Array
```

Index:	Name:	Value:	ValueUnits:
1	K1	0.5	

See Also

`addparameter`, `sbioparameter`

Purpose Parameter value units

Description The ValueUnits property indicates the unit definition of the parameter object Value property. ValueUnits can be one of the built-in units. To get a list of the built-in units, use the sbioshowunits function. If ValueUnits changes from one unit definition to another, the Value does not automatically convert to the new units. The sbioconvertunits function does this conversion.

You can add a parameter object to a model object or a kinetic law object.

Characteristics

Applies to	Object: parameter
Data type	char string
Data values	Unit from units library. Default is '' (empty).
Access	Read/write

Examples

Assign a parameter with a value to the model object.

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

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

- 2 Add a parameter with Value 0.5, and assign it to the model object (modelObj).

```
parameterObj1 = addparameter(modelObj, 'K1', 0.5, 'ValueUnits', '1/second')
```

MATLAB returns:

```
SimBiology Parameter Array
```

Index:	Name:	Value:	ValueUnits:
1	K1	0.5	1/second

See Also

addparameter, sbioconvertunits, sbioparameter, sbioshowunits

ZeroOrderDurationParameter

Purpose Zero order dose absorption duration

Description ZeroOrderDurationParameter is a property of the PKModelMap object. It specifies the name of an object that represents the duration of absorption when DoseType is zero-order. Specify the name of a parameter that is scoped to a model. When dosing multiple compartments, specify the parameters in the same order as the species in the Dosed property, with ' ' for compartments that are not dosed with zero-order kinetics. For an example, see “Dosing Multiple Compartments in a Model”.

Characteristics

Applies to	Objects: PKModelMap
Data type	char string or cell array of strings
Data values	Name of an object, or empty
Access	Read/write

See Also in the SimBiology User’s Guide, Estimated, Observed, PKModelMap object, DosingType

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