Package ‘rsbml’

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Description Links R to libsbml for SBML parsing, validating output, provides an S4 SBML DOM, converts SBML to R graph objects. Optionally links to the SBML ODE Solver Library (SOSLib) for simulating models.
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R topics documented:

AlgebraicRule-class .................................................. 2
AssignmentRule-class .............................................. 3
BoundingBox-class .................................................. 4
Compartment-class .................................................. 5
CompartmentGlyph-class .......................................... 7
CompartmentType-class ........................................... 8
CompartmentVolumeRule-class ................................. 9
Constraint-class ................................................... 10
CubicBezier-class .................................................. 11
Curve-class ........................................................ 12
CVTerm-class ......................................................... 13
Delay-class .......................................................... 14
describe .................................................................. 15
Dimensions-class .................................................... 15
Event-class ............................................................. 16
EventAssignment-class ............................................ 18
Experiment-class ...................................................... 19
FunctionDefinition-class ........................................... 20
## AlgebraicRule-class

*SBML type* "AlgebraicRule"

### Description

Expressions equations that are not assignments nor rates of change.
AssignmentRule-class

Instantiation

Objects can be created by calls of the form `new("AssignmentRule", ...)`.

Slots

- **math**: Object of class "expression" specifying the equation.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of `CVTerm` associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "Rule", directly. Class "SBase", by class "Rule", distance 2.

Methods

No methods defined with class "AssignmentRule" in the signature.

Author(s)

Michael Lawrence

References

[http://sbml.org/documents/](http://sbml.org/documents/)

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**AssignmentRule-class**  
**SBML type** "AssignmentRule"

Description

An equation that assigns a value to the quantity of a `Species`, the size of a `Compartment` or the value of a `Parameter`.

Instantiation

Objects can be created by calls of the form `new("AssignmentRule", ...)`.
Slots

variable: Object of class "character" naming the variable (the id of a Species, Compartment or Parameter) to set.
type: Object of class "character", deprecated.
math: Object of class "expression" specifying the equation.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "Rule", directly. Class "SBase", by class "Rule", distance 2.

Methods

variable signature(object = "AssignmentRule"): gets the variable slot
variable<- signature(object = "AssignmentRule"): sets the variable slot
type signature(object = "AssignmentRule"): gets the type slot
type<- signature(object = "AssignmentRule"): sets the type slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

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BoundingBox-class  SBML type "BoundingBox"

Description

Species the size and position of an SBML layout object.

Instantiation

Objects can be created by calls of the form new("BoundingBox", ...).
Slots

id: Object of class "character" uniquely identifying this component.
position: Object of class "Point" specifying the position.
dimensions: Object of class "Dimensions" specifying the size.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

id signature(object = "BoundingBox"): gets the id slot
id<- signature(object = "BoundingBox"): sets the id slot
dimensions signature(object = "BoundingBox"): gets the dimensions slot
dimensions<- signature(object = "BoundingBox"): sets the dimensions slot
position signature(object = "BoundingBox"): gets the position slot
position<- signature(object = "BoundingBox"): sets the position slot

Author(s)

Michael Lawrence

References

http://projects.villa-bosch.de/bcb/sbml
Slots

id: Object of class "character" uniquely identifying this component.
name: Object of class "character" naming this component.
spatialDimensions: Object of class "integer" indicating the number of dimensions (0, 1, 2, or 3)
size: Object of class "numeric" indicating the size in the given units.
units: Object of class "character" indicating the units (built-in or the id of a UnitDefinition).
outside: Object of class "character" identifying the compartment containing this compartment.
constant: Object of class "logical" indicating whether the size changes during simulation.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

id signature(object = "Compartment"): gets the id slot
id<- signature(object = "Compartment"): sets the id slot
name signature(object = "Compartment"): gets the name slot
name<- signature(object = "Compartment"): sets the name slot
constant signature(object = "Compartment"): gets the constant slot
constant<- signature(object = "Compartment"): sets the constant slot
outside signature(object = "Compartment"): gets the outside slot
outside<- signature(object = "Compartment"): sets the outside slot
size signature(object = "Compartment"): gets the size slot
size<- signature(object = "Compartment"): sets the size slot
units signature(object = "Compartment"): gets the constant slot
units<- signature(object = "Compartment"): sets the constant slot
spatialDimensions signature(object = "Compartment"): gets the spatialDimensions slot
spatialDimensions<- signature(object = "Compartment"): sets the spatialDimensions slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
CompartmentGlyph-class

SBML type "CompartmentGlyph"

Description

A glyph representing a Compartment.

Instantiation

Objects can be created by calls of the form `new("CompartmentGlyph", ...)`. 

Slots

- **compartment**: Object of class "character" identifying the compartment this glyph represents.
- **id**: Object of class "character" uniquely identifying this component.
- **boundingBox**: Object of class "BoundingBox" describing the position and size of the graphical object.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of CVTerm associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

Methods

- **compartment** signature(object = "CompartmentGlyph"): gets the compartment slot
- **compartment<-** signature(object = "CompartmentGlyph"): sets the compartment slot

Author(s)

Michael Lawrence

References

[http://projects.villa-bosch.de/bcb/sbml](http://projects.villa-bosch.de/bcb/sbml)
CompartmentType-class  

SBML Type "CompartmentType"

Description

Declares a type of Compartment. Compartments with the same type are logically similar.

Objects from the Class

Objects can be created by calls of the form new("CompartmentType", ...).

Slots

- id: Object of class "character" uniquely identifying this component.
- name: Object of class "character" naming this component.
- metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- notes: Object of class "character" containing user-readable XHTML notes about an element.
- annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
- sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

- id signature(object = "CompartmentType"): gets the id slot
- id<- signature(object = "CompartmentType"): sets the id slot
- name signature(object = "CompartmentType"): gets the name slot
- name<- signature(object = "CompartmentType"): sets the name slot

Note

Requires libsbml >= 3.0

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

See Also

Compartment
CompartmentVolumeRule-class

SBML type "CompartmentVolumeRule"

Description

Obsolete way to assign a volume to a Compartment.

Instantiation

Objects can be created by calls of the form new("CompartmentVolumeRule", ...).

Slots

- compartment: Object of class "character" identifying the compartment variable.
- variable: Object of class "character", ignored.
- type: Object of class "character", deprecated.
- math: Object of class "expression" specifying the equation.
- metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- notes: Object of class "character" containing user-readable XHTML notes about an element.
- annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
- sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends


Methods

- compartment signature(object = "CompartmentVolumeRule"): gets the compartment slot
- compartment<- signature(object = "CompartmentVolumeRule"): sets the compartment slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Constraint-class  

SBML Type "Constraint"

Description
A constraint that must be continuously satisfied throughout the simulation of a model. Once a constraint is no longer met, the simulation must halt.

Objects from the Class
Objects can be created by calls of the form `new("Constraint", ...)`. 

Slots
- `math`: Object of class "expression" that evaluates to `FALSE` if the constraint is not satisfied, otherwise evaluates to `TRUE`.
- `message`: Object of class "character", formatted in XHTML, that is displayed to the user by an application when the constraint is not satisfied.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends
Class "SBase", directly.

Methods

Note
Requires libsbml >= 3.0

Author(s)
Michael Lawrence

References
[http://sbml.org/documents/]
Description
A cubic bezier curve in an SBML layout.

Instantiation
Objects can be created by calls of the form `new("CubicBezier", ...)`.

Slots
- `basePoint1`: Object of class "Point" indicating the position of the base point closest to the starting point.
- `basePoint2`: Object of class "Point" indicating the position of the base point farthest from the starting point.
- `start`: Object of class "Point".
- `end`: Object of class "Point".
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends
Class "LineSegment", directly. Class "SBase", by class "LineSegment", distance 2.

Methods
- `basePoint1` signature(object = "CubicBezier"): gets the `basePoint1` slot
- `basePoint1<-` signature(object = "CubicBezier"): sets the `basePoint1` slot
- `basePoint2` signature(object = "CubicBezier"): gets the `basePoint2` slot
- `basePoint2<-` signature(object = "CubicBezier"): sets the `basePoint2` slot

Author(s)
Michael Lawrence

References
http://projects.villa-bosch.de/bcb/sbml
Curve-class

Description
A curve (list of line segments) in an SBML layout.

Instantiation
Objects can be created by calls of the form `new("Curve", ...)`.

Slots
- `curveSegments`: Object of class "list" containing the LineSegments that compose the curve.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of CVTerm associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends
Class "SBase", directly.

Methods
- `curveSegments` signature(object = "Curve"): gets the curveSegments slot
- `curveSegments<-` signature(object = "Curve"): sets the curveSegments slot

Author(s)
Michael Lawrence

References
http://projects.villa-bosch.de/bcb/sbml
CVTerm-class

SBML Type "CVTerm"

Description

A MIRIAM annotation, consisting of a qualifier ("model", "biological" or something else) and a resource (URI).

Objects from the Class

Objects can be created by calls of the form `new("CVTerm", ...)`.

Slots

- `qualifierType`: Object of class "character" specifying the type of qualifier for this term. Types "model" and "biological" have special meaning, but any string may be specified.
- `modelQualifierType`: Object of class "character" specifying the type of model qualifier, if `qualifierType` is set to "model". Types "is" and "isDescribedBy" are formally defined in MIRIAM, but any string may be specified.
- `biologicalQualifierType`: Object of class "character" specifying the type of biological qualifier, if `qualifierType` is set to "biological". Types "is", "hasPart", "isPartOf", "isVersionOf", "hasVersion", "isHomologTo", and "isDescribedBy" are formally defined in MIRIAM, though any string may be specified.
- `resources`: Object of class "character" specifying a URI that identifies some resource related an SBML element by the qualifier.

Methods

- `biologicalQualifierType` signature(object = "CVTerm"): gets the biologicalQualifierType slot.
- `biologicalQualifierType<-` signature(object = "CVTerm"): sets the biologicalQualifierType slot.
- `modelQualifierType` signature(object = "CVTerm"): gets the modelQualifierType slot.
- `modelQualifierType<-` signature(object = "CVTerm"): sets the modelQualifierType slot.
- `qualifierType` signature(object = "CVTerm"): gets the qualifierType slot.
- `qualifierType<-` signature(object = "CVTerm"): sets the qualifierType slot.
- `resources` signature(object = "CVTerm"): gets the resources slot.
- `resources<-` signature(object = "CVTerm"): sets the resources slot.

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Description

The length of time between the triggering of an Event and the execution of its EventAssignments.

Objects from the Class

Objects can be created by calls of the form new("Delay", ...).

Slots

math: Object of class "expression" that evaluates to a quantity of time.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

math signature(domain = "Delay"): gets the math slot.
math<- signature(object = "Delay"): sets the math slot.

Note

Requires libsbml >= 3.0

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

See Also

Event
Describe

Each class in the SBML DOM extends the Describable class and thus has a describe method, which describes an object with a short string. This is used by the show method to output terse textual representations of the DOM.

Usage

describe(object, ...)

Arguments

object The object to be described.
...
Additional arguments for methods.

Value

A short textual (string) representation of object.

Describable objects

An object that extends Describable has a method for the describe generic, and by default Describable objects are shown by printing the output of describe. Note that Describable is a virtual tag class, no objects may be created from it.

Describable methods

show signature(object = "Describable"): outputs the return value of describe.

Author(s)

Michael Lawrence

Dimensions-class SBML type "Dimensions"

Description

Holds the size of an SBML layout object.

Instantiation

Objects can be created by calls of the form new("Dimensions", ...).
Slots

width: Object of class "numeric" indicating the width, in pixels
height: Object of class "numeric" indicating the height, in pixels
depth: Object of class "numeric" indicating the depth, in pixels
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

depth signature(object = "Dimensions"): gets the depth slot
depth<- signature(object = "Dimensions"): sets the depth slot
height signature(object = "Dimensions"): gets the height slot
height<- signature(object = "Dimensions"): sets the height slot
width signature(object = "Dimensions"): gets the width slot
width<- signature(object = "Dimensions"): sets the width slot

Author(s)

Michael Lawrence

References

http://projects.villa-bosch.de/bcb/sbml

<table>
<thead>
<tr>
<th>Event-class</th>
<th>SBML type &quot;Event&quot;</th>
</tr>
</thead>
</table>

Description

Description of a instantaneous, discontinuous change in the model state.

Instantiation

Objects can be created by calls of the form new("Event", ...).
Slots

- **id**: Object of class "character" uniquely identifying this component.
- **name**: Object of class "character" naming this component.
- **trigger**: Object of class "expression" that evaluates to TRUE when the event is to be fired.
- **eventDelay**: Object of class "expression" that evaluates to the time until execution of this event after it has been fired.
- **timeUnits**: Object of class "character" identifying the units of the delay.
- **eventAssignments**: Object of class "list" containing EventAssignments that are performed at execution.
- **useValuesFromTriggerTime**: Object of class "logical". If FALSE, the event is evaluated after the delay, rather than when the event is executed.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of CVTerm associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

- **id** signature(object = "Event"): gets the id slot
- **id<-** signature(object = "Event"): sets the id slot
- **name** signature(object = "Event"): gets the name slot
- **name<-** signature(object = "Event"): sets the name slot
- **timeUnits** signature(object = "Event"): gets the timeUnits slot
- **timeUnits<-** signature(object = "Event"): sets the timeUnits slot
- **eventDelay** signature(x = "Event"): ...
- **eventDelay<-** signature(object = "Event"): sets the delay slot
- **eventAssignments** signature(object = "Event"): gets the eventAssignments slot
- **eventAssignments<-** signature(object = "Event"): sets the eventAssignments slot
- **trigger** signature(object = "Event"): gets the trigger slot
- **trigger<-** signature(object = "Event"): sets the trigger slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
EventAssignment-class  *SBML type* "EventAssignment"

**Description**

As part of an event, assigns a value to the quantity of a Species, the size of a Compartment or the value of a Parameter.

**Instantiation**

Objects can be created by calls of the form `new("EventAssignment", ...)`.  

**Slots**

- **variable**: Object of class "character" ~~
- **math**: Object of class "expression" that evaluates to the value to assign.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of CVTerm associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

**Extends**

Class "SBase", directly.

**Methods**

- `math signature(object = "EventAssignment")`: gets the math slot
- `math<- signature(object = "EventAssignment")`: sets the math slot
- `variable signature(object = "EventAssignment")`: gets the variable slot
- `variable<- signature(object = "EventAssignment")`: sets the variable slot

**Author(s)**

Michael Lawrence

**References**

[http://sbml.org/documents/]
Description

This class is an abstraction for an experiment, e.g. in a simulation. An experiment consists of a 
ExperimentProtocol, ExperimentDesign, ExperimentSubject and ExperimentResult.

Objects from the Class

A virtual Class: No objects may be created from it.

Slots

protocol: Object of empty virtual class ExperimentProtocol, how the experiment was or is to 
be performed.

design: Object of empty virtual class ExperimentDesign, the design of the experiment.

subject: Object of empty virtual class ExperimentSubject, the object being observed by the 
experiment.

result: Object of empty virtual class ExperimentResult, the result of the experiment.

Methods

\texttt{design} signature(object = "Experiment"): Gets the design slot.

\texttt{design}<- signature(object = "Experiment"): Sets the design slot.

\texttt{protocol} signature(object = "Experiment"): Gets the protocol slot.

\texttt{protocol}<- signature(object = "Experiment"): Sets the protocol slot.

\texttt{result} signature(object = "Experiment"): Gets the result slot.

\texttt{result}<- signature(object = "Experiment"): Sets the result slot.

\texttt{subject} signature(object = "Experiment"): Gets the subject slot.

\texttt{subject}<- signature(object = "Experiment"): Sets the subject slot.

Author(s)

Michael Lawrence

See Also

\texttt{SOSExperiment}, an implementation that simulates SBML modules using the SBML ODE Solver 
library.
FunctionDefinition-class

SBML type "FunctionDefinition"

Description

Identifies a mathematical expression so that it may be referenced in other expressions.

Instantiation

Objects can be created by calls of the form `new("FunctionDefinition", ...)`. 

Slots

- `id`: Object of class "character" uniquely identifying this component.
- `name`: Object of class "character" naming this component.
- `math`: Object of class "expression" that defines the function.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

- `id` signature(object = "FunctionDefinition"): gets the id slot
- `id<-` signature(object = "FunctionDefinition"): sets the id slot
- `name` signature(object = "FunctionDefinition"): gets the name slot
- `name<-` signature(object = "FunctionDefinition"): sets the name slot
- `math` signature(object = "FunctionDefinition"): gets the math slot
- `math<-` signature(object = "FunctionDefinition"): sets the math slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
GraphicalObject-class

GraphicalObject-class  SBML type "GraphicalObject"

Description

The base class for graphical objects (e.g. glyphs) in SBML layouts.

Instantiation

Objects can be created by calls of the form new("GraphicalObject", ...).

Slots

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

id signature(object = "GraphicalObject"): gets the id slot

id<- signature(object = "GraphicalObject"): sets the id slot

boundingBox signature(object = "GraphicalObject"): gets the boundingBox slot

boundingBox<- signature(object = "GraphicalObject"): sets the boundingBox slot

Author(s)

Michael Lawrence

References

http://projects.villa-bosch.de/bcb/sbml
InitialAssignment-class

SBML Type "InitialAssignment"

Description

Calculates the value of a symbol when the model is initialized.

Objects from the Class

Objects can be created by calls of the form `new("InitialAssignment", ...)`. 

Slots

- `symbol`: Object of class "character" to which the value is assigned.
- `math`: Object of class "expression" that evaluates to the assigned value.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

- `math` signature(object = "InitialAssignment"): gets the math slot.
- `math<-` signature(object = "InitialAssignment"): sets the math slot.
- `symbol` signature(object = "InitialAssignment"): gets the symbol slot.
- `symbol<-` signature(object = "InitialAssignment"): sets the symbol slot.

Note

Requires libsbml >= 3.0

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
**KineticLaw-class**

*See Also*

`AssignmentRule`, which can set a value at any time but cannot set constants.

---

**KineticLaw-class**  
*SBML type ”KineticLaw”*

**Description**

Describes the rate of a Reaction.

**Instantiation**

Objects can be created by calls of the form `new("KineticLaw", ...)`.

**Slots**

- `math`: Object of class "expression" defining the rate of the reaction.  
- `parameters`: Object of class "list" containing Parameters that may be used in `math`. The names of the list correspond to the IDs of the elements.  
- `timeUnits`: Object of class "character" indicating the units for time.  
- `substanceUnits`: Object of class "character" indicating the units for substance.  
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.  
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.  
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.  
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.  
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

**Extends**

Class "SBase", directly.

**Methods**

- `math signature(object = "KineticLaw")`: gets the `math` slot
- `math<- signature(object = "KineticLaw")`: sets the `math` slot
- `substanceUnits signature(object = "KineticLaw")`: gets the `substanceUnits` slot
- `substanceUnits<- signature(object = "KineticLaw")`: sets the `substanceUnits` slot
- `timeUnits signature(object = "KineticLaw")`: gets the `timeUnits` slot
- `timeUnits<- signature(object = "KineticLaw")`: sets the `timeUnits` slot
- `parameters signature(object = "KineticLaw")`: gets the `parameters` slot
- `parameters<- signature(object = "KineticLaw")`: sets the `parameters` slot
**Layout-class**

**Author(s)**

Michael Lawrence

**References**

http://sbml.org/documents/

---

**SBML type** "Layout"

**Description**

Contains the glyphs and other graphical objects that compose an SBML layout. Layouts are not part of the core SBML specification. See the reference for the SBML layout extension specification.

**Instantiation**

Objects can be created by calls of the form `new("Layout", ...)`. 

**Slots**

- **id**: Object of class "character" uniquely identifying this component.
- **dimensions**: Object of class "Dimensions" specifying the size of the layout.
- **compartmentGlyphs**: Object of class "list" containing the CompartmentGlyphs. The names of the list correspond to the IDs of the elements.
- **speciesGlyphs**: Object of class "list" containing the SpeciesGlyphs. The names of the list correspond to the IDs of the elements.
- **reactionGlyphs**: Object of class "list" containing the ReactionGlyphs. The names of the list correspond to the IDs of the elements.
- **textGlyphs**: Object of class "list" containing the TextGlyphs. The names of the list correspond to the IDs of the elements.
- **additionalGraphicalObjects**: Object of class "list" containing the additional GraphicalObjects that are not bound to any model component. The names of the list correspond to the IDs of the elements.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of CVTerm associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

**Extends**

Class "SBase", directly.
Methods

id signature(object = "Layout"): gets the id slot
id<- signature(object = "Layout"): sets the id slot

additionalGraphicalObjects signature(object = "Layout"): gets the additionalGraphicalObjects slot
additionalGraphicalObjects<- signature(object = "Layout"): sets the additionalGraphicalObjects slot

compartmentGlyphs signature(object = "Layout"): gets the compartmentGlyphs slot
compartmentGlyphs<- signature(object = "Layout"): sets the compartmentGlyphs slot
dimensions signature(object = "Layout"): gets the dimensions slot
dimensions<- signature(object = "Layout"): sets the dimensions slot
reactionGlyphs signature(object = "Layout"): gets the reactionGlyphs slot
reactionGlyphs<- signature(object = "Layout"): sets the reactionGlyphs slot

speciesGlyphs signature(object = "Layout"): gets the speciesGlyphs slot
speciesGlyphs<- signature(object = "Layout"): sets the speciesGlyphs slot
textGlyphs signature(object = "Layout"): gets the textGlyphs slot
textGlyphs<- signature(object = "Layout"): sets the textGlyphs slot

Author(s)

Michael Lawrence

References

http://projects.villa-bosch.de/bcb/sbml

LineSegment-class  SBML type "LineSegment"

Description

Describes a simple A-B line.

Instantiation

Objects can be created by calls of the form new("LineSegment", ...).

Slots

start: Object of class "Point" indicating the start position.
end: Object of class "Point" indicating the end position.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends
Class "SBase", directly.

Methods
end signature(x = "LineSegment"): ...
end <- signature(object = "LineSegment"): sets the end slot
start signature(x = "LineSegment"): ...
start <- signature(object = "LineSegment"): sets the start slot

Author(s)
Michael Lawrence

References
http://projects.villa-bosch.de/bcb/sbml

MathML Utilities

Description
Each of these functions implements a trigonometry function found in the MathML specification but not found in base R. These are all simple wrappers around existing R trig functions.

Usage
acot(x)
acoth(x)
acsc(x)
acsch(x)
asec(x)
asech(x)
cot(x)
coth(x)
csc(x)
csch(x)
sec(x)
sech(x)

Arguments
x The numeric value(s) for the trigonometry operation
**Model-class**

**Value**

A numeric vector, the same length as x.

**Author(s)**

Michael Lawrence

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**Description**

The central SBML element. Contains the Species, Reactions, Compartments and other components of the model. See the SBML specification, at the reference, for further details.

**Instantiation**

Objects can be created by calls of the form `new("Model", ...)`.

**Slots**

- **id**: Object of class "character" uniquely identifying this component.
- **name**: Object of class "character" naming this component.
- **functionDefinitions**: Object of class "list" containing FunctionDefinitions. The names of the list correspond to the IDs of the elements.
- **unitDefinitions**: Object of class "list" containing UnitDefinitions. The names of the list correspond to the IDs of the elements.
- **compartments**: Object of class "list" containing Compartments. The names of the list correspond to the IDs of the elements.
- **species**: Object of class "list" containing Species. The names of the list correspond to the IDs of the elements.
- **parameters**: Object of class "list" containing Parameters. The names of the list correspond to the IDs of the elements.
- **rules**: Object of class "list" containing Rules.
- **reactions**: Object of class "list" containing Reactions. The names of the list correspond to the IDs of the elements.
- **events**: Object of class "list" containing Events. The names of the list correspond to the IDs of the elements.
- **layouts**: Object of class "list" containing Layouts. The names of the list correspond to the IDs of the elements.
- **speciesTypes**: Object of class "list" containing SpeciesTypes. The names of the list correspond to the IDs of the elements.
- **compartmentTypes**: Object of class "list" containing CompartmentTypes. The names of the list correspond to the IDs of the elements.
- **constraints**: Object of class "list" containing Constraints. The names of the list correspond to the IDs of the elements.
Model-class

initialAssignments: Object of class "list" containing InitialAssignments.
modelHistory: Object of class ModelHistory recording the history of the model.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This
links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element,
but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information
about an element, usually as RDF, such as BioPAX. This is where application-specific data
belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends
Class "SBase", directly.

Methods

id signature(object = "Model"): gets the id slot
id<- signature(object = "Model"): sets the id slot
name signature(object = "Model"): gets the name slot
name<- signature(object = "Model"): sets the name slot
compartments signature(object = "Model"): gets the compartments slot
compartments<- signature(object = "Model"): sets the compartments slot
events signature(object = "Model"): gets the events slot
events<- signature(object = "Model"): sets the events slot
functionDefinitions signature(object = "Model"): gets the functionDefinitions slot
functionDefinitions<- signature(object = "Model"): sets the functionDefinitions slot
layouts signature(object = "Model"): gets the layouts slot
layouts<- signature(object = "Model"): sets the layouts slot
parameters signature(object = "Model"): gets the parameters slot
parameters<- signature(object = "Model"): sets the parameters slot
species signature(object = "Model"): gets the species slot
species<- signature(object = "Model"): sets the species slot
reactions signature(object = "Model"): gets the reactions slot
reactions<- signature(object = "Model"): sets the reactions slot
rules signature(object = "Model"): gets the rules slot
rules<- signature(object = "Model"): sets the rules slot
unitDefinitions signature(object = "Model"): gets the unitDefinitions slot
unitDefinitions<- signature(object = "Model"): sets the unitDefinitions slot
compartmentTypes signature(object = "Model"): gets the compartmentTypes slot
compartmentTypes<- signature(object = "Model"): sets the compartmentTypes slot
constraints signature(object = "Model"): gets the constraints slot
ModelCreator-class

**constraints<-** signature(object = "Model"): sets the constraints slot

**initialAssignments** signature(object = "Model"): gets the initialAssignments slot

**initialAssignments<-** signature(object = "Model"): sets the initialAssignments slot

**speciesTypes** signature(object = "Model"): gets the speciesTypes slot

**speciesTypes<-** signature(object = "Model"): sets the speciesTypes slot

**modelHistory** signature(object = "Model"): gets the modelHistory slot

**modelHistory<-** signature(object = "Model"): sets the modelHistory slot

**stoichiometryMatrix** signature(object = "Model"): calculates the stoichiometry matrix of the model

**Author(s)**

Michael Lawrence

**References**

[http://sbml.org/documents/](http://sbml.org/documents/)

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**ModelCreator-class**

**SBML Type** "ModelCreator"

**Description**

Information, such as name, email and organization, about a creator of an SBML model.

**Objects from the Class**

Objects can be created by calls of the form `new("ModelCreator", ...)`. 

**Slots**

- **familyName**: Object of class "character" specifying the family name of the creator.
- **givenName**: Object of class "character" specifying the given name of the creator.
- **email**: Object of class "character" specifying the email address of the creator.
- **organization**: Object of class "character" specifying the name of the organization to which the creator belongs.

**Methods**

- **email** signature(object = "ModelCreator"): gets the email slot.
- **email<-** signature(object = "ModelCreator"): sets the email<- slot.
- **familyName** signature(object = "ModelCreator"): gets the familyName slot.
- **familyName<-** signature(object = "ModelCreator"): sets the familyName<- slot.
- **givenName** signature(object = "ModelCreator"): gets the givenName slot.
- **givenName<-** signature(object = "ModelCreator"): sets the givenName<- slot.
- **organization** signature(object = "ModelCreator"): gets the organization slot.
- **organization<-** signature(object = "ModelCreator"): sets the organization<- slot.
ModelHistory-class

Author(s)
Michael Lawrence

References
http://sbml.org/documents/

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ModelHistory-class  SBML Type "ModelHistory"

Description
Stores the history of an SBML model, including the created/modified dates and the creators.

Objects from the Class
Objects can be created by calls of the form new("ModelHistory", ...).

Slots
createdDate: Object of class "character" representing the date/time of creation, in W3CDTF format: YYYY-MM-DDTh:mm:ssTZD, e.g. "1997-07-16T19:20:30+01:00".
modifiedDate: Object of class "character" representing the date/time of last modification, in W3CDTF format: YYYY-MM-DDTh:mm:ssTZD, e.g. "1997-07-16T19:20:30+01:00".
creators: Object of class "list" of instances of ModelCreator, one for each creator of the model.

Methods
createdDate signature(object = "ModelHistory"): get the createdDate slot.
createdDate<- signature(object = "ModelHistory", value = "character"): Set the createdDate slot to a correctly formatted string.
createdDate<- signature(object = "ModelHistory", value = "POSIXt"): Set the createdDate slot with a POSIXt instance, obtained e.g. from Sys.time.
creators signature(object = "ModelHistory"): gets the creators slot.
creators<- signature(object = "ModelHistory"): sets the creators slot.
modifiedDate signature(object = "ModelHistory"): get the modifiedDate slot.
modifiedDate<- signature(object = "ModelHistory", value = "character"): Set the modifiedDate slot to a correctly formatted string.
modifiedDate<- signature(object = "ModelHistory", value = "POSIXt"): Set the modifiedDate slot with a POSIXt instance, obtained e.g. from Sys.time.

Author(s)
Michael Lawrence

References
http://sbml.org/documents/
Description

Identifies a Species that modifies the parent Reaction.

Instantiation

Objects can be created by calls of the form new("ModifierSpeciesReference", ...).

Slots

id: Object of class "character" uniquely identifying this component.
species: Object of class "character" identifying the Species being referenced.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends


Methods

No methods defined with class "ModifierSpeciesReference" in the signature.

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Parameter-class

SBML type "Parameter"

Description

Declares a variable to be used in a mathematical expression.

Instantiation

Objects can be created by calls of the form `new("Parameter", ...)`.

Slots

- **id**: Object of class "character" uniquely identifying this component.
- **name**: Object of class "character" naming this component.
- **value**: Object of class "numeric" specifying the initial value.
- **units**: Object of class "character" identifying the units.
- **constant**: Object of class "logical" indicating whether the value of this parameter is constant.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of `CVTerm` associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

- `id` signature(object = "Parameter"): gets the id slot
- `id<-` signature(object = "Parameter"): sets the id slot
- `name` signature(object = "Parameter"): gets the name slot
- `name<-` signature(object = "Parameter"): sets the name slot
- `units` signature(object = "Parameter"): gets the units slot
- `units<-` signature(object = "Parameter"): sets the units slot
- `constant` signature(object = "Parameter"): gets the constant slot
- `constant<-` signature(object = "Parameter"): sets the constant slot
- `value` signature(object = "Parameter"): gets the value slot
- `value<-` signature(object = "Parameter"): sets the value slot
**ParameterRule-class**

**Author(s)**

Michael Lawrence

**References**

http://sbml.org/documents/

---

**Description**

**Obsolete** rule that controls the value of a Parameter.

**Instantiation**

Objects can be created by calls of the form `new("ParameterRule", ...)`.  

**Slots**

- `name`: Object of class "character" naming this component.
- `units`: Object of class "character" identifying the units of the assigned value.
- `variable`: Object of class "character", ignored.
- `type`: Object of class "character", deprecated.
- `math`: Object of class "expression" specifying the equation.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

**Extends**

Class "**AssignmentRule**", directly. Class "**Rule**", by class "**AssignmentRule**", distance 2. Class "**SBase**", by class "**AssignmentRule**", distance 3.

**Methods**

- `name signature(object = "Parameter")`: gets the name slot
- `name<- signature(object = "Parameter")`: sets the name slot
- `units signature(object = "Parameter")`: gets the units slot
- `units<- signature(object = "Parameter")`: sets the units slot
- `variable signature(object = "Parameter")`: gets the variable slot
variables-< signature(object = "Parameter"): sets the variable slot
type signature(object = "Parameter"): gets the type slot
type<- signature(object = "Parameter"): sets the type slot
math signature(object = "Parameter"): gets the math slot
math<- signature(object = "Parameter"): sets the math slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

---

Point-class  SBML type "Point"

Description

Specifies a position in 3D space.

Instantiation

Objects can be created by calls of the form new("Point", ...).

Slots

x: Object of class "numeric" indicating the X coordinate
y: Object of class "numeric" indicating the Y coordinate
z: Object of class "numeric" indicating the Z coordinate
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.
RateRule-class

Methods

x signature(object = "Point"): gets the x slot
x<- signature(object = "Point"): sets the x slot
y signature(object = "Point"): gets the y slot
y<- signature(object = "Point"): sets the y slot
z signature(object = "Point"): gets the z slot
z<- signature(object = "Point"): sets the z slot

Author(s)

Michael Lawrence

References

http://projects.villa-bosch.de/bcb/sbml

RateRule-class

SBML type "RateRule"

Description

An equation that describes the rate of change in the quantity of a Species, the size of a Compartment or the value of a Parameter.

Instantiation

Objects can be created by calls of the form new("RateRule", ...).

Slots

variable: Object of class "character" naming the variable (the id of a Species, Compartment or Parameter) being described.

math: Object of class "expression" specifying the equation.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "Rule", directly. Class "SBase", by class "Rule", distance 2.
Methods

```r
variable signature(object = "RateRule"): gets the variable slot
variable<- signature(object = "RateRule"): sets the variable slot
```

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

---

**Reaction-class**

*SBML type* "Reaction"

---

**Description**

Any transformation, transportation or binding process that changes the quantity of one or more *Species*.

**Instantiation**

Objects can be created by calls of the form `new("Reaction", ...)`.

**Slots**

- **id**: Object of class "character" uniquely identifying this component.
- **name**: Object of class "character" naming this component.
- **reactants**: Object of class "list" containing *SpeciesReferences* specifying the *Species* that are reactants for this reaction. The names of the list correspond to the IDs of the species.
- **products**: Object of class "list" containing *SpeciesReferences* specifying the *Species* that are products for this reaction. The names of the list correspond to the IDs of the species.
- **modifiers**: Object of class "list" containing *ModifierSpeciesReferences* specifying the *Species* that are modifiers for this reaction. The names of the list correspond to the IDs of the species.
- **kineticLaw**: Object of class "KineticLaw" that dynamically defines the rate of the reaction.
- **reversible**: Object of class "logical" indicating whether the direction of this reaction is reversible.
- **fast**: Object of class "logical" indicating whether this reaction should be considered instantaneous relative to non-fast reactions.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the *annotation* element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of *CVTerm* associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).
Extends

Class "SBase", directly.

Methods

- `id` signature(object = "Reaction"): gets the id slot
- `id<-` signature(object = "Reaction"): sets the id slot
- `name` signature(object = "Reaction"): gets the name slot
- `name<-` signature(object = "Reaction"): sets the name slot
- `fast` signature(object = "Reaction"): gets the fast slot
- `fast<-` signature(object = "Reaction"): sets the fast slot
- `kineticLaw` signature(object = "Reaction"): gets the kineticLaw slot
- `kineticLaw<-` signature(object = "Reaction"): sets the kineticLaw slot
- `modifiers` signature(object = "Reaction"): gets the modifiers slot
- `modifiers<-` signature(object = "Reaction"): sets the modifiers slot
- `products` signature(object = "Reaction"): gets the products slot
- `products<-` signature(object = "Reaction"): sets the products slot
- `reactants` signature(object = "Reaction"): gets the reactants slot
- `reactants<-` signature(object = "Reaction"): sets the reactants slot
- `reversible` signature(object = "Reaction"): gets the reversible slot
- `reversible<-` signature(object = "Reaction"): sets the reversible slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Slots

reaction: Object of class "character" identifying the reaction represented by this glyph.
glyphCurve: Object of class "Curve" describing this glyph as a curve (optional).
speciesReferenceGlyphs: Object of class "list" containing SpeciesReferenceGlyphs that represent the SpeciesReferences of the underlying Reaction. The names of the list correspond to the IDs of the elements.
id: Object of class "character" uniquely identifying this component.
boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

Methods

glyphCurve signature(expr = "ReactionGlyph"): gets the glyphCurve slot
glyphCurve<- signature(object = "ReactionGlyph"): sets the glyphCurve slot
reaction signature(object = "ReactionGlyph"): gets the reaction slot
reaction<- signature(object = "ReactionGlyph"): sets the reaction slot
speciesReferenceGlyphs signature(object = "ReactionGlyph"): gets the speciesReferenceGlyphs slot
speciesReferenceGlyphs<- signature(object = "ReactionGlyph"): sets the speciesReferenceGlyphs slot

Author(s)

Michael Lawrence

References

http://projects.villa-bosch.de/bcb/sbml
Description

A mathematical equation.

Instantiation

A virtual Class: No objects may be created from it.

Slots

- **math**: Object of class "expression" specifying the equation.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of CVTerm associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

- **math** signature(object = “Rule”): gets the math slot
- **math<-** signature(object = “Rule”): sets the math slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
SBML type "SBase"

Description

The abstract type from which all other SBML types are derived.

Instantiation

A virtual Class: No objects may be created from it.

Slots

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Methods

annotation signature(object = "SBase"): gets the annotation slot

annotation<- signature(object = "SBase"): sets the annotation slot

metaId signature(object = "SBase"): gets the metaId slot

metaId<- signature(object = "SBase"): sets the metaId slot

notes signature(object = "SBase"): gets the notes slot

notes<- signature(object = "SBase"): sets the notes slot

cvTerms signature(object = "SBase"): gets the cvTerms slot.

cvTerms<- signature(object = "SBase"): sets the cvTerms slot.

sboTerm signature(object = "SBase"): gets the sboTerm slot.

sboTerm<- signature(object = "SBase"): sets the sboTerm slot.

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
**SBML import**

**Description**

Read an SBML file into R.

**Usage**

```
rsbml_read(filename, text, dom = TRUE, strict = FALSE, schema = FALSE,
            consistency = TRUE)
```

**Arguments**

- `filename`: the name of the SBML file to parse
- `text`: a string of SBML text to parse (instead of file)
- `dom`: whether to convert directly to the S4 DOM (TRUE, the default) or leave as the internal `SBMLDocument`
- `strict`: whether to report warnings in addition to errors or not (FALSE, the default)
- `schema`: whether to perform XML schema validation
- `consistency`: whether to perform consistency checks; recommended but might cause performance deficiencies.

**Value**

A `SBML` object, or a `SBMLDocument` if `dom` is FALSE.

**Author(s)**

Michael Lawrence

**Examples**

```r
# Read an SBML file
file <- system.file("sbml", "GlycolysisLayout.xml", package = "rsbml")
doc <- rsbml_read(file)

# Read an SBML string
string <- paste(readLines(file), collapse = "\n")
doc <- rsbml_read(text = string)
```
SBML-class

SBML type "SBML"

Description

The root element of an SBML document. An actual SBML Model may be retrieved from an instance of this class.

Instantiation

Objects can be created by calls of the form `new("SBML", ...)

Slots

`level`: Object of class "integer" indicating the level of the SBML standard (currently at 2).
`ver`: Object of class "integer" indicating the version of the level (currently at 2 for level 2).
`model`: Object of class "Model" the SBML model itself.
`metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
`notes`: Object of class "character" containing user-readable XHTML notes about an element.
`annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
`cvTerms`: Object of class "list" containing instances of CVTerm associated with this element.
`sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

`coerce` signature(from = "SBMLDocument", to = "SBML"): constructs the S4 object model from a low-level libsbml document.
`coerce` signature(from = "SBML", to = "SBMLDocument"): converts the S4 object model to a low-level libsbml document.
`coerce` signature(from = "SBML", to = "graph"): converts the S4 object model to a graph.
`level` signature(object = "SBML"): gets the level slot
`level<-` signature(object = "SBML"): sets the level slot
`model` signature(object = "SBML"): gets the model slot
`model<-` signature(object = "SBML"): sets the model slot
`rsbml\_doc` signature(model = "SBML"): converts the S4 object model to a low-level libsbml document.
`rsbml\_write` signature(object = "SBML"): writes this document to a file as SBML.
`rsbml\_xml` signature(object = "SBML"): converts this document to a string as SBML.
`rsbml_graph` signature(object = "SBML"): converts this document to a graph object.

`rsbml_check` signature(object = "SBML"): perform consistency checks, see `rsbml_check`.

`simulate` signature(object = "SBML"): converts this document to an internal `SBMLDocument` and calls `simulate` on it.

`ver` signature(object = "SBML"): gets the ver slot

`ver<-` signature(object = "SBML"): sets the ver slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

Examples

```r
# Get a DOM
dom <- rsbml_read(system.file("sbml", "GlycolysisLayout.xml", package = "rsbml"))

# Get the species ID's
sapply(species(model(dom)), id)

# Convert DOM back to a low-level document for checking
doc <- rsbml_doc(dom)
rsbml_check(doc)

# Write a DOM to a file
## Not run: rsbml_write(dom, "my.xml")
```

---

**SBMLDocument-class**

"SBMLDocument" from libsbml

**Description**

Low-level libsbml document structure.

**Instantiation**

A virtual Class: No objects may be created from it.

**Extends**

Class "oldClass", directly.
Methods

rsbml\_check signature(object = "SBMLDocument"): \texttt{rsbml\_check(object, strict = FALSE, consistency = TRUE)}: Check for problems with the document and signal R conditions if any errors are detected. If \texttt{strict} is \texttt{TRUE}, \texttt{libsbml} warnings will be emitted as R warnings (these are often too pedantic). If \texttt{consistency} is also \texttt{TRUE}, reports problems regarding internal model inconsistencies. This can be time consuming.

rsbml\_dom signature(doc = "SBMLDocument"): Constructs an S4 object model from a libsbml document.

rsbml\_graph signature(doc = "SBMLDocument"): Converts a libsbml document to a graph.

rsbml\_problems signature(object = "SBMLDocument"): reports problems encountered during parsing and/or validation.

rsbml\_write signature(object = "SBMLDocument"): writes this problems to a file as SBML.

rsbml\_xml signature(object = "SBMLDocument"): converts this document to a string as SBML.

simulate signature(object = "SBMLDocument"): simulate(object, nsim = 10, seed, ...): a shortcut for simulating the model in this document using the SBML ODE Solver library. Arguments in ... should match slots of \texttt{SOSProtocol}. See simulate for more details.

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

Examples

# Read a document into an R DOM
\texttt{dom} <- \texttt{rsbml\_read(system.file("sbml", "GlycolysisLayout.xml", package = "rsbml"))}

# Convert to a graph
\texttt{graph} <- \texttt{rsbml\_graph(dom)}

# Write it out to a file
## Not run: \texttt{rsbml\_write(dom, "my.xml")}

# Or convert it to a string of XML
\texttt{rsbml\_xml(dom)}

# Read into external libsbml data structure
\texttt{doc} <- \texttt{rsbml\_read(system.file("sbml", "GlycolysisLayout.xml", package = "rsbml"), dom = FALSE)}

# Convert it explicitly to an S4 DOM
\texttt{dom} <- \texttt{rsbml\_dom(doc)}
**SBMLProblem-class**

**SBMLProblem**

**Description**

Represents an exception thrown during SBML parsing.

**Details**

There are trivial subclasses for fatal errors (SBMLFatal), recoverable errors (SBLError), warnings (SBMLWarning) and informational messages (SBMLInfo). Errors become R error conditions, warnings become R warning conditions and messages are output via message.

**Slots**

- **line**: The "numeric" line number in the SBML file where the problem was detected.
- **column**: Object of class "numeric" column number in the SBML file where the problem was detected.
- **msg**: Object of class "character", a human-readable description of the problem.

**Methods**

- **.condition** signature(object = "SBMLProblem"): constructs a condition object representing the exception.

**Author(s)**

Michael Lawrence

**See Also**

[SBMLProblems](#), a container for instances of this class.

---

**SBMLProblems-class**

**SBMLProblems**

**Description**

A class representing errors encountered during parsing of SBML.

**Slots**

- **fatal**: A list of SBMLFatal instances.
- **error**: A list of SBLError instances.
- **warning**: A list of SBMLWarning instances.
- **info**: A list of SBMLInfo instances.
Methods

.throw signature(object = "SBMLProblems"): Throws each \texttt{SBMLProblem} in this object.
.errors signature(object = "SBMLProblems"): Gets the \texttt{errors} slot.
.fatals signature(object = "SBMLProblems"): Gets the \texttt{fatals} slot.
.infos signature(object = "SBMLProblems"): Gets the \texttt{infos} slot.
.warns signature(object = "SBMLProblems"): Gets the \texttt{warns} slot.

Author(s)

Michael Lawrence

See Also

The \texttt{rsbml_problems} function for obtaining an instance of this class describing any problems encountered during parsing.

---

**SimpleSpeciesReference-class**

\textit{SBML type "SimpleSpeciesReference"}

Description

Base class for bindings between a \textit{Species} and a \textit{Reaction}.

Instantiation

Objects can be created by calls of the form \texttt{new("SimpleSpeciesReference", ...)}.

Slots

- \texttt{id}: Object of class "character" uniquely identifying this component.
- \texttt{species}: Object of class "character" identifying the \textit{Species} being referenced.
- \texttt{metaId}: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the \texttt{annotation} element.
- \texttt{notes}: Object of class "character" containing user-readable XHTML notes about an element.
- \texttt{annotation}: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- \texttt{cvTerms}: Object of class "list" containing instances of \texttt{CVTerm} associated with this element.
- \texttt{sboTerm}: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "\texttt{SBase}", directly.
Methods

id signature(object = "SpeciesGlyph"): gets the id slot
id<- signature(object = "SpeciesGlyph"): sets the id slot

species signature(object = "SpeciesGlyph"): gets the species slot
species<- signature(object = "SpeciesGlyph"): sets the species slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

| SOSDesign-class | SOSDesign |

Description

Specifies the reaction names and their parameter settings for each run in a batch experiment. It extends matrix; each column corresponds to a parameter in the model and each row should hold the parameter settings for one run of the experiment.

Details

It is often desirable to explore the state space of a model by adjusting its initial parameter settings. One could do this by modifying the model itself for each experiment, but this class aims to provide a more convenient and systematic means of running experiments in batch, over a range of parameter settings. The results of the experiment will then contain the output from each run, which may then be compared.

The design is specified as a matrix, and each column in the matrix should correspond to a parameter defined in an SBML model. The column names should identify the parameters. These are not to be confused with the simulation parameters specified in SOSProtocol, which control how the simulation is executed. These should be and are designed to be kept constant across the runs.

There are two different types of parameters: global and local (reaction) parameters. Global parameters may correspond to a Species quantity, Compartment size, or model-level Parameter value. These should be identified in the column names by the id of the corresponding SBML element. The element in the reactions slot for one of these parameters should be the empty string.

The second type of parameter specifies the value of a Parameter element within the KineticLaw of a reaction. These should be named by the id of the Parameter. They also should be named by the containing Reaction id, which is stored in the corresponding element of the reactions slot.

Objects from the Class

Objects can be created by calls of the form new("SOSDesign", data, nrow, ncol, byrow, dimnames, ...). This is the same as initializing a matrix.
SOSExperiment-class

Slots

(Util: Object of class "matrix", holding the parameter settings.
reactions: Object of class "character" of length the number of columns, holding the reaction IDs for parameters local to a reaction (i.e. KineticLaw Parameters). For global parameters, the corresponding value should be the empty string.

Extends


Methods

reactions signature(object = "SOSDesign"): gets the reactions slot.
reactions<- signature(object = "SOSDesign"): sets the reactions slot.

Author(s)

Michael Lawrence

References

See http://www.tbi.univie.ac.at/~raim/odeSolver/ for more information on the SBML ODE Solver library.

See Also

SOSExperiment, the container of this class, for configuring and running a simulation.

---

SOSExperiment-class  SOS Experiment

Description

Implementation of Experiment for simulating SBML models using the SOS: (S)BML (O)DE (S)olver library.

Details

The general workflow for running a simulation:

1. Create or import an SBML DOM.
2. Customize the model, for example by adding perturbation Events.
3. Wrap the SBML DOM in a SOSSubject, e.g. new("SOSSubject", dom).
4. Optionally construct a SOSDesign for running the experiment in batch over several sets of model parameter settings.
5. Optionally construct a SOSProtocol for specifying the time points and other parameters controlling the simulation.
6. Construct an instance of this class that groups the subject, design and protocol.
7. Run `simulate` on the `SOSExperiment`, optionally specifying the number of iterations and the random seed.

8. Analyze the returned `SOSResult`, perhaps starting by converting it to a time series with `as.ts` and making some plots.

**Objects from the Class**

Objects can be created by calls of the form `new("SOSExperiment", ...)`.

**Slots**

- `protocol`: Object of class `SOSProtocol`, where the simulation parameters are specified.
- `design`: Object of class `SOSDesign`, specifying model parameters for each run of a batch experiment.
- `subject`: Object of class `SOSSubject`, containing the `Model` to be simulated.
- `result`: Object of class `SOSResult` containing the result of the simulation.

**Extends**

Class `Experiment`, directly.

**Methods**

- `simulate` signature(`object = "SOSExperiment")`: `simulate(object, nsim = 10, seed, ...)`: Simulates the SBML document in the `subject` slot according to the design points in `design` and parameters in `protocol` for `nsim` iterations, using `seed` as the random seed. Returns an instance of `SOSExperiment`, which now should include a `SOSResult` for analysis.

**Author(s)**

Michael Lawrence

**References**


**See Also**

The `simulate` method on `SBMLDocument` is a shortcut, but most users will probably find the above approach most useful.
**SOSProtocol-class**

**Description**

Holds the parameters controlling the execution of the simulation using the SBML ODE Solver library.

**Details**

Most users will probably set only the `times` slot, either directly or through the `timeStep` slot and the `nsim` parameter to `simulate`.

**Objects from the Class**

Objects can be created by calls of the form `new("SOSProtocol", ...)`. Each argument in ... should correspond to one of the slots described below.

**Slots**

- `times`: A "numeric" vector indicating the time points at which to evaluate the model. Defaults to `tail(seq(0, by = timeStep, length.out = nsim + 1), -1)`. The model is always evaluated at `t = 0`. This slot is ignored when `indefinite` (below) is `TRUE`. 
- `timeStep`: A scalar "numeric" value, giving the length in time between model evaluations. This is used when calculating the default value of `times`, above, but is otherwise only relevant when the `indefinite` slot, below, is `TRUE`. Defaults to 1.
- `indefinite`: A scalar "logical", indicating whether the simulation should run indefinitely, i.e. until one of the stopping conditions is met. See `haltOnEvent` and `haltOnSteadyState` below. Defaults to `FALSE`.
- `atol`: Scalar "numeric", the absolute tolerance in integration error. Defaults to `1e-18`.
- `rtol`: Scalar "numeric", the relative tolerance in integration error. Defaults to `1e-10`.
- `maxStep`: Scalar "numeric", the maximum number of steps for integration. Not to be confused with `timeStep`, etc, above, which control the simulation time points. Defaults to `10000`.
- `odeMethod`: Scalar "character" naming the method for solving ODEs. Either "bdf" (the default) or "adams-moulton".
- `iterMethod`: Scalar "character", naming the iteration method used by the ODE solver, either "newton" (the default) or "functional".
- `maxOrder`: Scalar "numeric" indicating maximum order for the ODE solver. Defaults to 5.
- `sensMethod`: Scalar "character" naming the method for sensitivity analysis. One of "none" (the default and currently the only valid option), "simultaneous", "staggered" or "staggered1".
- `haltOnEvent`: Scalar "logical" indicating whether the simulation should halt when the model emits an `Event`. This allows the model to stop the simulation when some state is reached. Defaults to `FALSE`.
- `haltOnSteadyState`: Scalar "logical", indicating whether to halt when a steady state is detected. Defaults to `FALSE`.
- `useJacobian`: Scalar "logical" indicating whether to use Jacobian ASTs (TRUE, the default) or the internal approximation in the CVODES library.
- `storeResults`: Scalar "logical" indicating whether to store the entire time course (TRUE, the default) or just the last time point. Just for performance.
SOSResult-class

Extends

Class "ExperimentProtocol", directly.

Methods

No methods defined with class "SOSProtocol" in the signature.

Author(s)

Michael Lawrence

References

See http://www.tbi.univie.ac.at/~raim/odeSolver/ for more information on the SBML ODE Solver library.

See Also

The SOSExperiment class, which contains a SOSProtocol instance, for setting up and running a simulation.

SOSResult-class

Description

A result from simulating an SOSExperiment. Contains the time course for each of the model variables: the Species quantities, Compartment sizes, Parameter values, and Reaction rates.

Slots

data: A "data.frame" containing the time course data. Each row contains the value at a single time point for a single time course. Has the following columns:

  sample  A factor, the run number, only exists if there were multiple runs, see SOSDesign.
  type    A factor, the SBML element type for the time course, e.g. "species".
  id      A factor, the id of the SBML element for the time course.
  time    The numeric time value for the time point.
  value   The actual numeric value for the time course at that time.
  sens: A "matrix" with results from sensitivity analysis, not yet supported.

Extends

Class "ExperimentResult", directly.
SOSSubject-class

Methods

**as.ts** signature(x = "SOSResult"): converts this object to a time course object of class ts. This allows analysis of the results with existing R infrastructure for time course analysis.

**compartments** signature(object = "SOSResult"): returns a subset containing only the **Compartment** size courses.

**parameters** signature(object = "SOSResult"): returns a subset containing only the global **Parameter** value courses.

**reactions** signature(object = "SOSResult"): returns a subset containing only the **Reaction** rate courses.

**species** signature(object = "SOSResult"): returns a subset containing only the **Species** quantity courses.

Author(s)

Michael Lawrence

References


See Also

**SOSExperiment** for running a simulation and obtaining an instance of this class.

---

SOSSubject-class  SOSSubject

Description

This just marks an **SBML** object as being a valid subject for simulation using the SBML ODE Solver library.

Objects from the Class

Normally created from a SBML with: `new("SOSSubject", model).

Extends

Class "**ExperimentSubject**", directly. Class "**SBML**", directly. Class "**SBase**", by class "SBML", distance 2. Class "**Describable**", by class "SBML", distance 3.

Author(s)

Michael Lawrence

References

Species-class

See Also

SOSExperiment for running a simulation on a SOSSubject.

Species-class  SBML type "Species"

Description

A participant in an SBML model.

Instantiation

Objects can be created by calls of the form new("Species", ...).

Slots

id: Object of class "character" uniquely identifying this component.
name: Object of class "character" naming this component.
compartment: Object of class "character" identifying the compartment in which this species is located.
initialAmount: Object of class "numeric" indicating the initial amount for this species (mutually exclusive with initialConcentration).
initialConcentration: Object of class "numeric" indicating the initial concentration for this species (mutually exclusive with initialAmount).
substanceUnits: Object of class "character" identifying the units for the amount of this species or the numerator of the concentration.
spatialSizeUnits: Object of class "character" identifying the units for the denominator of the species concentration.
hasOnlySubstanceUnits: Object of class "logical" indicating whether the quantity of this species is specified as an amount or a concentration.
boundaryCondition: Object of class "logical". If TRUE, indicates that the quantity of this species cannot be changed by a reaction.
charge: Object of class "integer" indicating the electrical charge of this species.
constant: Object of class "logical" indicating whether the quantity of this species can change.
units: Object of class "character", deprecated.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).
Species-class

Extends

Class "SBase", directly.

Methods

id signature(object = "Species"): gets the id slot
id<- signature(object = "Species"): sets the id slot
name signature(object = "Species"): gets the name slot
name<- signature(object = "Species"): sets the name slot
boundaryCondition signature(object = "Species"): gets the boundaryCondition slot
boundaryCondition<- signature(object = "Species"): sets the boundaryCondition slot
charge signature(object = "Species"): gets the charge slot
charge<- signature(object = "Species"): sets the charge slot
compartment signature(object = "Species"): gets the compartment slot
compartment<- signature(object = "Species"): sets the compartment slot
constant signature(object = "Species"): gets the constant slot
constant<- signature(object = "Species"): sets the constant slot
units signature(object = "Species"): gets the constant slot
units<- signature(object = "Species"): sets the constant slot
hasOnlySubstanceUnits signature(object = "Species"): gets the hasOnlySubstanceUnits slot
hasOnlySubstanceUnits<- signature(object = "Species"): sets the hasOnlySubstanceUnits slot
initialAmount signature(object = "Species"): gets the initialAmount slot
initialAmount<- signature(object = "Species"): sets the initialAmount slot
initialConcentration signature(object = "Species"): gets the initialConcentration slot
initialConcentration<- signature(object = "Species"): sets the initialConcentration slot
spatialSizeUnits signature(object = "Species"): gets the spatialSizeUnits slot
spatialSizeUnits<- signature(object = "Species"): sets the spatialSizeUnits slot
substanceUnits signature(object = "Species"): gets the substanceUnits slot
substanceUnits<- signature(object = "Species"): sets the substanceUnits slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Description

**Obsolete** type of rule that describes the concentration of Species.

Instantiation

Objects can be created by calls of the form `new("SpeciesConcentrationRule", ...)`.

Slots

- `species`: Object of class "character" identifying the Species.
- `variable`: Object of class "character", ignored.
- `type`: Object of class "character", deprecated.
- `math`: Object of class "expression" specifying the equation.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of CVTerm associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends


Methods

- `species` signature(object = "SpeciesConcentrationRule"): gets the species slot
- `species<-` signature(object = "SpeciesConcentrationRule"): sets the species slot

Author(s)

Michael Lawrence

References

[http://sbml.org/documents/](http://sbml.org/documents/)
SpeciesGlyph-class  

SBML type "SpeciesGlyph"

Description

A glyph representing a Species in an SBML layout.

Instantiation

Objects can be created by calls of the form `new("SpeciesGlyph", ...)`.

Slots

- `species`: Object of class "character" identifying the species this glyph represents.
- `id`: Object of class "character" uniquely identifying this component.
- `boundingBox`: Object of class "BoundingBox" describing the position and size of the graphical object.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

Methods

- `species` signature(object = "SpeciesGlyph"): gets the species slot
- `species<-` signature(object = "Species Glyph"): sets the species slot

Author(s)

Michael Lawrence

References

[http://projects.villa-bosch.de/bcb/sbml](http://projects.villa-bosch.de/bcb/sbml)
SpeciesReference-class

SBML type "SpeciesReference"

Description

Binds a reactant or product Species to a Reaction.

Instantiation

Objects can be created by calls of the form new("SpeciesReference", ...).

Slots

stoichiometry: Object of class "numeric" indicating the (static) stoichiometric coefficient.
stoichiometryMath: Object of class "StoichiometryMath" that dynamically calculates the stoichiometric coefficient.
id: Object of class "character" uniquely identifying this component.
species: Object of class "character" identifying the Species being referenced.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends


Methods

stoichiometry signature(object = "SpeciesReference"): gets the stoichiometry slot
stoichiometry<- signature(object = "SpeciesReference"): sets the stoichiometry slot
stoichiometryMath signature(object = "SpeciesReference"): gets the stoichiometryMath slot
stoichiometryMath<- signature(object = "SpeciesReference"): sets the stoichiometryMath slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Description

A glyph representing a SpeciesReference in an SBML layout.

Instantiation

Objects can be created by calls of the form new("SpeciesReferenceGlyph", ...).

Slots

speciesGlyph: Object of class "character" identifying the SpeciesGlyph representing the Species that is referenced by the underlying SpeciesReference.

speciesReference: Object of class "character" identifying the linkS4class{SpeciesReference} represented by this glyph.

role: Object of class "character" indicating how this glyph should represent the "role" of the underlying SpeciesReference.

glyphCurve: Object of class "Curve" describing this glyph as a curve (optional).

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.

Methods

role signature(object = "SpeciesReferenceGlyph"): gets the role slot

role<- signature(object = "SpeciesReferenceGlyph"): sets the role slot

speciesGlyph signature(object = "SpeciesReferenceGlyph"): gets the speciesGlyph slot

speciesGlyph<- signature(object = "SpeciesReferenceGlyph"): sets the speciesGlyph slot

speciesReference signature(object = "SpeciesReferenceGlyph"): gets the speciesReference slot
SpeciesType-class

- **speciesReference**: sets the speciesReference slot
- **glyphCurve**: gets the glyphCurve slot
- **glyphCurve**: sets the glyphCurve slot

Author(s)
Michael Lawrence

References
http://projects.villa-bosch.de/bcb/sbml

---

SpeciesType-class  SBML Type "SpeciesType"

Description
A Species represents a pool of a chemical in a particular linkS4class(Compartment). This element specifies a type of species, that is, the chemical independent of location.

Objects from the Class
Objects can be created by calls of the form `new("SpeciesType", ...)`.

Slots
- **id**: Object of class "character" uniquely identifying this component.
- **name**: Object of class "character" naming this component.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of CVTerm associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends
Class "SBase", directly.

Methods
- **id**: gets the id slot
- **id**: sets the id slot
- **name**: gets the name slot
- **name**: sets the name slot
Note
Requires libsbml >= 3.0

Author(s)
Michael Lawrence

References
http://sbml.org/documents/

See Also
Species

StoichiometryMath-class

SBML type "StoichiometryMath"

Description
Dynamically defines the stoichiometry of a SpeciesReference.

Instantiation
Objects can be created by calls of the form new("StoichiometryMath", ...).

Slots
math: Object of class "expression" that evaluates to the stoichiometric coefficient.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends
Class "SBase", directly.

Methods
math signature(object = "StoichiometryMath"): gets the math slot
math<- signature(object = "StoichiometryMath"): sets the math slot
TextGlyph-class

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

TextGlyph-class  SBML type "TextGlyph"

Description

A run of text in an SBML layout.

Instantiation

Objects can be created by calls of the form new("TextGlyph", ...).

Slots

graphicalObject: Object of class "character" identifying the GraphicalObject that this glyph labels (optional).

text: Object of class "character" containing the text shown by the glyph (mutually exclusive with originOfText).

originOfText: Object of class "character" identifying an SBML component whose name is used as the text (mutually exclusive with text).

id: Object of class "character" uniquely identifying this component.

boundingBox: Object of class "BoundingBox" describing the position and size of the graphical object.

metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.

notes: Object of class "character" containing user-readable XHTML notes about an element.

annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.

cvTerms: Object of class "list" containing instances of CVTerm associated with this element.

sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "GraphicalObject", directly. Class "SBase", by class "GraphicalObject", distance 2.
Methods

- **graphicalObject** signature(object = "TextGlyph"): gets the graphicalObject slot
- **graphicalObject**<- signature(object = "TextGlyph"): sets the graphicalObject slot
- **originOfText** signature(object = "TextGlyph"): gets the originOfText slot
- **originOfText**<- signature(object = "TextGlyph"): sets the originOfText slot
- **text** signature(x = "TextGlyph"): ...
- **text**<- signature(object = "TextGlyph"): sets the text slot

Author(s)

Michael Lawrence

References

http://projects.villa-bosch.de/bcb/sbml

---

**Trigger-class**  
**SBML Type "Trigger"**

Description

Expresses when an Event should be fired.

Objects from the Class

Objects can be created by calls of the form `new("Trigger", ...)`.

Slots

- **math**: Object of class "expression" that evaluates to TRUE when the event should be fired.
- **metaId**: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- **notes**: Object of class "character" containing user-readable XHTML notes about an element.
- **annotation**: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- **cvTerms**: Object of class "list" containing instances of **CVTerm** associated with this element.
- **sboTerm**: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "SBase", directly.

Methods

- **math** signature(domain = "Trigger"): gets the math slot.
- **math**<- signature(object = "Trigger"): sets the math slot.
**Unit-class**

**Note**
Requires libsbml >= 3.0

**Author(s)**
Michael Lawrence

**References**
http://sbml.org/documents/

**See Also**
*Event*, the parent of this element.

---

**Unit-class**  
*SBML type "Unit"*

**Description**
A (possibly transformed) reference to a base UnitKind. The transformation is of the form: \( \text{multiplier} \times 10^{\text{scale}} \times x^{\text{exponent}} + \text{offset} \).

**Instantiation**
Objects can be created by calls of the form `new("Unit", ...)`.

**Slots**
- `kind`: Object of class "character" identifying a an SBML UnitKind. For possible values see Table 2 in the SBML specification.
- `exponent`: Object of class "integer" indicating the exponent to use in the transformation.
- `unitScale`: Object of class "integer" indicating the order of magnitude of the scaling to use in the transformation.
- `multiplier`: Object of class "numeric" indicating the factor to use for scaling in the transformation.
- `offset`: Object of class "numeric" indicating the amount of constant shift in the transformation.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the `annotation` element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of `CVTerm` associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).
Extends

Class "SBase", directly.

Methods

\begin{verbatim}
exponent signature(object = "Unit"): gets the exponent slot
exponent<- signature(object = "Unit"): sets the exponent slot
kind signature(object = "Unit"): gets the kind slot
kind<- signature(object = "Unit"): sets the kind slot
multiplier signature(object = "Unit"): gets the multiplier slot
multipliers<- signature(object = "Unit"): sets the multiplier slot
offset signature(object = "Unit"): gets the offset slot
offset<- signature(object = "Unit"): sets the offset slot
unitScale signature(x = "Unit"): ...
unitScale<- signature(object = "Unit"): sets the unitScale slot
\end{verbatim}

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

\begin{verbatim}
UnitDefinition-class  SBML type "UnitDefinition"
\end{verbatim}

Description

Associates one or more Units with an ID and name.

Instantiation

Objects can be created by calls of the form new("UnitDefinition", ...).

Slots

id: Object of class "character" uniquely identifying this component.
name: Object of class "character" naming this component.
units: Object of class "list" containing equivalent Units that are all associated with the same ID and name.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.
annotation: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
cvTerms: Object of class "list" containing instances of CVTerm associated with this element.
sboTerm: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).
Extends

Class "SBase", directly.

Methods

- \texttt{id} signature(object = "UnitDefinition"): gets the \texttt{id} slot
- \texttt{id<-} signature(object = "UnitDefinition"): sets the \texttt{id} slot
- \texttt{name} signature(object = "UnitDefinition"): gets the \texttt{name} slot
- \texttt{name<-} signature(object = "UnitDefinition"): sets the \texttt{name} slot
- \texttt{units} signature(object = "UnitDefinition"): gets the \texttt{units} slot
- \texttt{units<-} signature(object = "UnitDefinition"): sets the \texttt{units} slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Index

*Topic IO
SBML import, 41

*Topic classes
AlgebraicRule-class, 2
AssignmentRule-class, 3
BoundingBox-class, 4
Compartment-class, 5
CompartmentGlyph-class, 7
CompartmentType-class, 8
CompartmentVolumeRule-class, 9
Constraint-class, 10
CubicBezier-class, 11
Curve-class, 12
CVTerm-class, 13
Delay-class, 14
describe, 15
Dimensions-class, 15
Event-class, 16
EventAssignment-class, 18
Experiment-class, 19
FunctionDefinition-class, 20
GraphicalObject-class, 21
InitialAssignment-class, 22
KineticLaw-class, 23
Layout-class, 24
LineSegment-class, 25
Model-class, 27
ModelCreator-class, 29
ModelHistory-class, 30
ModifierSpeciesReference-class, 31
Parameter-class, 32
ParameterRule-class, 33
Point-class, 34
RateRule-class, 35
Reaction-class, 36
ReactionGlyph-class, 37
Rule-class, 39
SBase-class, 40
SBML-class, 42
SBMLDocument-class, 43
SBMLProblem-class, 45
SBMLProblems-class, 45
SimpleSpeciesReference-class, 46
SOSDesign-class, 47
SOSExperiment-class, 48
SOSPprotocol-class, 50
SOSResult-class, 51
SOSSubject-class, 52
Species-class, 53
SpeciesConcentrationRule-class, 55
SpeciesGlyph-class, 56
SpeciesReference-class, 57
SpeciesReferenceGlyph-class, 58
SpeciesType-class, 59
StoichiometryMath-class, 60
TextGlyph-class, 61
Trigger-class, 62
Unit-class, 63
UnitDefinition-class, 64

*Topic math
math, 26
.acot (math), 26
.acoth (math), 26
.acsc (math), 26
.acsch (math), 26
.additionalGraphicalObjects (Layout-class), 24
.additionalGraphicalObjects, Layout-method (Layout-class), 24
.additionalGraphicalObjects<-(Layout-class), 24
.additionalGraphicalObjects<-,Layout-method (Layout-class), 24
.AlgebraicRule-class, 2
INDEX

annotation (SBase-class), 40
annotation, SBase-method (SBase-class), 40
annotation<- (SBase-class), 40
annotation<-, SBase-method (SBase-class), 40
array, 48
as.character.SBML (SBML-class), 42
as.character.SBMLDocument (SBMLDocument-class), 43
as.ts, 49
as.ts, SOSResult-method (SOSResult-class), 51
asec (math), 26
asech (math), 26
AssignmentRule, 9, 23, 33, 55
AssignmentRule-class, 3
basePoint1 (CubicBezier-class), 11
basePoint1, CubicBezier-method (CubicBezier-class), 11
basePoint1<-, CubicBezier-class, 11
basePoint1<-, CubicBezier-method (CubicBezier-class), 11
basePoint2 (CubicBezier-class), 11
basePoint2, CubicBezier-method (CubicBezier-class), 11
basePoint2<-, CubicBezier-class, 11
basePoint2<-, CubicBezier-method (CubicBezier-class), 11
biologicalQualifierType (CVTerm-class), 13
biologicalQualifierType, CVTerm-method (CVTerm-class), 13
biologicalQualifierType<-, CVTerm-class, 13
biologicalQualifierType<-, CVTerm-method (CVTerm-class), 13
boundaryCondition (Species-class), 53
boundaryCondition, Species-method (Species-class), 53
boundaryCondition<-, Species-class, 53
boundaryCondition<-, Species-method (Species-class), 53
boundingBox (GraphicalObject-class), 21
boundingBox, GraphicalObject-method (GraphicalObject-class), 21
BoundingBox-class, 4
boundingBox<-, GraphicalObject-class, 21
boundingBox<-, GraphicalObject-method (GraphicalObject-class), 21
charge (Species-class), 53
charge, Species-method (Species-class), 53
charge<-, Species-class, 53
charge<-, Species-method (Species-class), 53
coerce (SBML-class), 42
coerce, SBML, graph-method (SBML-class), 42
coerce, SBMLDocument, graph-method (SBMLDocument-class), 42
coerce, SBMLDocument, graph-method (SBMLDocument-class), 43
coerce, SBMLDocument, SBML-method (SBMLDocument-class), 43
Compartment, 3, 4, 7–9, 18, 27, 35, 47, 51, 52
compartment (Species-class), 53
compartment, CompartmentGlyph-method (CompartmentGlyph-class), 7
compartment, CompartmentVolumeRule-method (CompartmentVolumeRule-class), 9
compartment, Species-method (Species-class), 53
Compartment-class, 5
compartment<-, Species-class, 53
compartment<-, CompartmentGlyph-method (CompartmentGlyph-class), 7
compartment<-, CompartmentVolumeRule-method (CompartmentVolumeRule-class), 9
compartment<-, Species-method (Species-class), 53
CompartmentGlyph, 24
CompartmentGlyph-class, 7
compartmentGlyphs (Layout-class), 24
compartmentGlyphs, Layout-method (Layout-class), 24
compartmentGlyphs<-, Layout-class, 24
compartmentGlyphs<-, Layout-method (Layout-class), 24
compartments (Model-class), 27
compartments, Model-method (Model-class), 27
compartments, SOSResult-method (SOSResult-class), 51
compartments<-, Model-class, 27
compartments<-, Model-method (Model-class), 27
CompartmentType, 27
CompartmentType-class, 8
compartmentTypes (Model-class), 27
INDEX

compartmentTypes, Model-method (Model-class), 27
compartmentTypes<-(Model-class), 27
compartmentTypes<-, Model-method (Model-class), 27
CompartmentVolumeRule-class, 9
condition, 45
constant (Species-class), 53
constant, Compartment-method (Compartment-class), 5
constant, Parameter-method (Parameter-class), 32
constant, Species-method (Species-class), 53
constant<-, (Species-class), 53
constant<-, Compartment-method (Compartment-class), 5
constant<-, Parameter-method (Parameter-class), 32
constant<-, Species-method (Species-class), 53
Constraint, 27
Constraint-class, 10
constraints (Model-class), 27
constraints, Model-method (Model-class), 27
constraints<-(Model-class), 27
constraints<-, Model-method (Model-class), 27
cot (math), 26
coth (math), 26
createdDate (ModelHistory-class), 30
createdDate, ModelHistory-method (ModelHistory-class), 30
createdDate<-(ModelHistory-class), 30
createdDate<-, ModelHistory, character-method (ModelHistory-class), 30
createdDate<-, ModelHistory, POSIXt-method (ModelHistory-class), 30
creators (ModelHistory-class), 30
creators, ModelHistory-method (ModelHistory-class), 30
creators<-(ModelHistory-class), 30
creators<-, ModelHistory-method (ModelHistory-class), 30
csc (math), 26
csch (math), 26
CubicBezier-class, 11
Curve-class, 12
curveSegments (Curve-class), 12
curveSegments, Curve-method (Curve-class), 12
curveSegments<-(Curve-class), 12
curves, Curve-method (Curve-class), 12
CVTerm, 3–12, 14, 16–18, 20–24, 26, 28, 31–36, 38–40, 42, 46, 53, 55–64
CVTerm-class, 13
cvTerms (SBase-class), 40
cvTerms, SBase-method (SBase-class), 40
cvTerms<-(SBase-class), 40
cvTerms<-, SBase-method (SBase-class), 40
Delay-class, 14
depth (Dimensions-class), 15
depth, Dimensions-method (Dimensions-class), 15
depth<-(Dimensions-class), 15
depth<-, Dimensions-method (Dimensions-class), 15
Describable, 52
Describable-class (describe), 15
describe, 15, 15
describe, AlgebraicRule-method (describe), 15
describe, AssignmentRule-method (describe), 15
describe, BoundingBox-method (describe), 15
describe, Compartment-method (describe), 15
describe, CompartmentGlyph-method (describe), 15
describe, CompartmentType-method (describe), 15
describe, CompartmentVolumeRule-method (describe), 15
describe, Constraint-method (describe), 15
describe, CubicBezier-method (describe), 15
describe, Curve-method (describe), 15
describe, CVTerm-method (describe), 15
describe, Delay-method (describe), 15
describe, Dimensions-method (describe), 15
describe, Event-method (describe), 15
describe, EventAssignment-method (describe), 15
describe, FunctionDefinition-method (describe), 15
describe, GraphicalObject-method (describe), 15
describe, InitialAssignment-method (describe), 15
ExperimentSubject, 52
ExperimentSubject-class (Experiment-class), 19
exponent (Unit-class), 63
exponent,Unit-method (Unit-class), 63
exponent<- (Unit-class), 63
exponent<-,Unit-method (Unit-class), 63

familyName (ModelCreator-class), 29
familyName,ModelCreator-method (ModelCreator-class), 29
familyName<- (ModelCreator-class), 29
familyName<-,ModelCreator-method (ModelCreator-class), 29

fast (Reaction-class), 36
fast,Reaction-method (Reaction-class), 36
fast<- (Reaction-class), 36
fast<-,Reaction-method (Reaction-class), 36

fatals (SBMLProblems-class), 45
fatals,SBMLProblems-method (SBMLProblems-class), 45

FunctionDefinition, 27
FunctionDefinition-class, 20
functionDefinitions (Model-class), 27
functionDefinitions,Model-method (Model-class), 27
functionDefinitions<- (Model-class), 27
functionDefinitions<-,Model-method (Model-class), 27

givenName (ModelCreator-class), 29
givenName,ModelCreator-method (ModelCreator-class), 29
givenName<- (ModelCreator-class), 29
givenName<-,ModelCreator-method (ModelCreator-class), 29
glyphCurve (ReactionGlyph-class), 37
glyphCurve,ReactionGlyph-method (ReactionGlyph-class), 37
glyphCurve,SpeciesReferenceGlyph-method (SpeciesReferenceGlyph-class), 58
glyphCurve<- (ReactionGlyph-class), 37
glyphCurve<-,ReactionGlyph-method (ReactionGlyph-class), 37
glyphCurve<-,SpeciesReferenceGlyph-method (SpeciesReferenceGlyph-class), 58

graph, 44
GraphicalObject, 7, 24, 38, 56, 58, 61
graphicalObject (TextGlyph-class), 61
graphicalObject,TextGlyph-method (TextGlyph-class), 61
GraphicalObject-class, 21
graphicalObject<- (TextGlyph-class), 61
graphicalObject<-,TextGlyph-method (TextGlyph-class), 61

hasOnlySubstanceUnits (Species-class), 53
hasOnlySubstanceUnits,Species-method (Species-class), 53
hasOnlySubstanceUnits<- (Species-class), 53
hasOnlySubstanceUnits<-,Species-method (Species-class), 53

height (Dimensions-class), 15
height,Dimensions-method (Dimensions-class), 15
height<- (Dimensions-class), 15
height<-,Dimensions-method (Dimensions-class), 15

id (UnitDefinition-class), 64
id,BoundingBox-method (BoundingBox-class), 4
id,Compartment-method (Compartment-class), 5
id,CompartmentType-method (CompartmentType-class), 8
id,Event-method (Event-class), 16
id,FunctionDefinition-method (FunctionDefinition-class), 20
id,GraphicalObject-method (GraphicalObject-class), 21
id,Layout-method (Layout-class), 24
id,Model-method (Model-class), 27
id,Parameter-method (Parameter-class), 32
id,Reaction-method (Reaction-class), 36
id,SimpleSpeciesReference-method (SimpleSpeciesReference-class), 46
id,Species-method (Species-class), 53
id,SpeciesType-method (SpeciesType-class), 59
id,UnitDefinition-method (UnitDefinition-class), 64
id<- (UnitDefinition-class), 64
id<-,BoundingBox-method (BoundingBox-class), 4
id<-,Compartment-method (Compartment-class), 5
id<-, CompartmentType-method (CompartmentType-class), 8
id<-, Event-method (Event-class), 16
id<-, FunctionDefinition-method (FunctionDefinition-class), 20
id<-, GraphicalObject-method (GraphicalObject-class), 21
id<-, Layout-method (Layout-class), 24
id<-, Model-method (Model-class), 27
id<-, Parameter-method (Parameter-class), 32
id<-, Reaction-method (Reaction-class), 36
id<-, SimpleSpeciesReference-method (SimpleSpeciesReference-class), 46
id<-, Species-method (Species-class), 53
id<-, SpeciesType-method (SpeciesType-class), 59
id<-, UnitDefinition-method (UnitDefinition-class), 64
initialAmount (Species-class), 53
initialAmount<-, Species-method (Species-class), 53
initialAssignments (Model-class), 27
initialAssignments<-, Model-method (Model-class), 27
initialConcentration (Species-class), 53
initialConcentration<-, Species-method (Species-class), 53
InitialAssignment, 28
InitialAssignment-class, 22
InitialAssignments (Model-class), 27
InitialAssignments, Model-method (Model-class), 27
InitialAssignments<-, Model-method (Model-class), 27
initialConcentration (Species-class), 53
initialConcentration<-, Species-method (Species-class), 53
initialConcentration<-, Species-method (Species-class), 53
kind (Unit-class), 63
kind, Unit-method (Unit-class), 63
kind<-, Unit-method (Unit-class), 63
KineticLaw, 47, 48
KineticLaw (Reaction-class), 36
kineticLaw, Reaction-method (Reaction-class), 36
KineticLaw-class, 23
kineticLaw<-, Reaction-method (Reaction-class), 36
LineSegment, 11, 12
LineSegment-class, 25
Layout, 27
Layout-class, 24
layouts, Model-method (Model-class), 27
layout<-, Model-method (Model-class), 27
level (SBML-class), 42
level, SBML-method (SBML-class), 42
level<-, SBML-method (SBML-class), 42
LineSegment, 11, 12
LineSegment-class, 25
math, 26
math (KineticLaw-class), 23
math, Constraint-method (Constraint-class), 10
math, Delay-method (Delay-class), 14
math, EventAssignment-method (EventAssignment-class), 18
math, FunctionDefinition-method (FunctionDefinition-class), 20
math, InitialAssignment-method (InitialAssignment-class), 22
math, KineticLaw-method (KineticLaw-class), 23
math, ParameterRule-method (ParameterRule-class), 33
math, Rule-method (Rule-class), 39
math, StoichiometryMath-method (StoichiometryMath-class), 60
math, Trigger-method (Trigger-class), 62
math<-, KineticLaw-class, 23
math<-, Constraint-method (Constraint-class), 10
math<-, Delay-method (Delay-class), 14
math<-, EventAssignment-method (EventAssignment-class), 18
math<-, FunctionDefinition-method (FunctionDefinition-class), 20
math<-, InitialAssignment-method (InitialAssignment-class), 22
math<-, KineticLaw-method (KineticLaw-class), 23
math<-, ParameterRule-method (ParameterRule-class), 33
notes, SBase-method (SBase-class), 40
notes<-, SBase-method (SBase-class), 40
offset (Unit-class), 63
offset, Unit-method (Unit-class), 63
offset<-, (Unit-class), 63
offset<-, Unit-method (Unit-class), 63
oldClass, 43
OptionalCurve-class (Curve-class), 12
OptionalDelay-class (Delay-class), 14
OptionalKineticLaw-class
  (KineticLaw-class), 23
OptionalModelHistory-class
  (ModelHistory-class), 30
OptionalStoichiometryMath-class
  (StoichiometryMath-class), 60
organization, ModelCreator-method (ModelCreator-class), 29
organization, ModelCreator-method (ModelCreator-class), 29
organization<-, ModelCreator-method (ModelCreator-class), 29
originOfText (TextGlyph-class), 61
originOfText, TextGlyph-method (TextGlyph-class), 61
originOfText<-, TextGlyph-method (TextGlyph-class), 61
originOfText<-, TextGlyph-method (TextGlyph-class), 61
outside (Compartment-class), 5
outside, Compartment-method (Compartment-class), 5
outside<-, (Compartment-class), 5
outside<-, Compartment-method (Compartment-class), 5

Parameter, 3, 4, 18, 23, 27, 33, 35, 47, 48, 51, 52
Parameter-class, 32
ParameterRule-class, 33
parameters (Model-class), 27
parameters, KineticLaw-method (KineticLaw-class), 23
parameters, Model-method (Model-class), 27
parameters, SOSResult-method (SOSResult-class), 51
parameters<-, (Model-class), 27
parameters<-, KineticLaw-method (KineticLaw-class), 23
parameters<-, Model-method (Model-class), 27
Point-class, 34
position (BoundingBox-class), 4
position, BoundingBox-method (BoundingBox-class), 4
position<-, BoundingBox-method (BoundingBox-class), 4
position<-, BoundingBox-class (BoundingBox-class), 4
POSIX, 30
products (Reaction-class), 36
products, Reaction-method (Reaction-class), 36
products<-, Reaction-method (Reaction-class), 36
products<-, Reaction-method (Reaction-class), 36
protocol (Experiment-class), 19
protocol (Experiment-class), 19
protocol<-, (Experiment-class), 19
protocol<-, (Experiment-class), 19

qualifierType (CVTerm-class), 13
qualifierType, CVTerm-method (CVTerm-class), 13
qualifierType<-, CVTerm-method (CVTerm-class), 13

RateRule-class, 35
reactants (Reaction-class), 36
reactants, Reaction-method (Reaction-class), 36
reactants<-, (Reaction-class), 36
reactants<-, Reaction-method (Reaction-class), 36
Reaction, 23, 27, 31, 37, 38, 46, 51, 52, 57
reaction (ReactionGlyph-class), 37
reaction, ReactionGlyph-method (ReactionGlyph-class), 37
Reaction-class, 36
reaction<-, (ReactionGlyph-class), 37
reaction<-, ReactionGlyph-method (ReactionGlyph-class), 37
ReactionGlyph, 24
ReactionGlyph-class, 37
reactionGlyphs (Layout-class), 24
reactionGlyphs, Layout-method (Layout-class), 24
reactionGlyphs<-, (Layout-class), 24
reactionGlyphs<-, Layout-method (Layout-class), 24
reactions (Model-class), 27
reactions, Model-method (Model-class), 27
<table>
<thead>
<tr>
<th>Term</th>
<th>Page(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>simulate</td>
<td>44, 50</td>
</tr>
<tr>
<td>simulate (SOSExperiment-class)</td>
<td>48</td>
</tr>
<tr>
<td>simulate, SBML-method (SBML-class)</td>
<td>42</td>
</tr>
<tr>
<td>simulate, SBMLDocument-method (SBMLDocument-class)</td>
<td>43</td>
</tr>
<tr>
<td>simulate, SOSExperiment-method (SOSExperiment-class)</td>
<td>48</td>
</tr>
<tr>
<td>size (Compartment-class)</td>
<td>5</td>
</tr>
<tr>
<td>size&lt;-, Compartment-method</td>
<td>(Compartment-class), 5</td>
</tr>
<tr>
<td>size&lt;- (Compartment-class)</td>
<td>5</td>
</tr>
<tr>
<td>size&lt;-, Compartment-method</td>
<td>(Compartment-class), 5</td>
</tr>
<tr>
<td>SOSDesign</td>
<td>48, 49, 51</td>
</tr>
<tr>
<td>SOSDesign-class</td>
<td>47</td>
</tr>
<tr>
<td>SOSExperiment</td>
<td>19, 48, 51–53</td>
</tr>
<tr>
<td>SOSExperiment-class</td>
<td>48</td>
</tr>
<tr>
<td>SOSPResult</td>
<td>44, 47–49</td>
</tr>
<tr>
<td>SOSPResult-class</td>
<td>50</td>
</tr>
<tr>
<td>SOSResult</td>
<td>49</td>
</tr>
<tr>
<td>SOSResult-class</td>
<td>51</td>
</tr>
<tr>
<td>SOSSubject</td>
<td>48, 49</td>
</tr>
<tr>
<td>SOSSubject-class</td>
<td>52</td>
</tr>
<tr>
<td>spatialDimensions (Compartment-class)</td>
<td>5</td>
</tr>
<tr>
<td>spatialDimensions&lt;-, Compartment-method</td>
<td>(Compartment-class), 5</td>
</tr>
<tr>
<td>spatialDimensions&lt;-, Compartment-method</td>
<td>(Compartment-class), 5</td>
</tr>
<tr>
<td>spatialSizeUnits (Species-class)</td>
<td>53</td>
</tr>
<tr>
<td>spatialSizeUnits, Species-method</td>
<td>(Species-class), 53</td>
</tr>
<tr>
<td>spatialSizeUnits&lt;- (Species-class)</td>
<td>53</td>
</tr>
<tr>
<td>spatialSizeUnits&lt;- (Species-method)</td>
<td>(Species-class), 53</td>
</tr>
<tr>
<td>Species, 3–5, 18, 27, 31, 35, 36, 46, 47, 51, 52, 55–60</td>
<td></td>
</tr>
<tr>
<td>species (SpeciesGlyph-class)</td>
<td>56</td>
</tr>
<tr>
<td>species, Model-method (Model-class)</td>
<td>27</td>
</tr>
<tr>
<td>species, SimpleSpeciesReference-method</td>
<td>(SimpleSpeciesReference-class), 46</td>
</tr>
<tr>
<td>species, SOSResult-method (SOSResult-class)</td>
<td>51</td>
</tr>
<tr>
<td>species, SpeciesConcentrationRule-method (SpeciesConcentrationRule-class)</td>
<td>55</td>
</tr>
<tr>
<td>species, SpeciesGlyph-method (SpeciesGlyph-class)</td>
<td>56</td>
</tr>
<tr>
<td>Species-class</td>
<td>53</td>
</tr>
<tr>
<td>species&lt;-, SpeciesGlyph-class</td>
<td>56</td>
</tr>
</tbody>
</table>