# Package 'rsbml'

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Title R support for SBML, using libsbml

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Imports BiocGenerics, graph, utils

SystemRequirements libsbml (==5.10.2)

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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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AlgebraicRule-class SBML type "AlgebraicRule"

### Description

Expresses equations that are not assignments nor rates of change.

# Instantiation

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

# 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 "AlgebraicRule" in the signature.

# Author(s)

Michael Lawrence

### References

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</pre>

# Author(s)

Michael Lawrence

### References

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 positon.

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</pre>

# Author(s)

Michael Lawrence

#### References

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

Compartment-class SBML type "Compartment"

# Description

A bounded space that contains Species.

### Instantiation

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

# 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</pre> 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</pre>

# 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</pre>

# Author(s)

Michael Lawrence

# References

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</pre> CompartmentVolumeRule-class

# Note

Requires libsbml  $\geq 3.0$ 

# 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: 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

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

### 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

math signature(domain = "Constraint"): gets the math slot.
math<- signature(object = "Constraint"): sets the math slot.
msg signature(domain = "Constraint"): gets the msg slot.
msg<- signature(object = "Constraint"): sets the msg slot.</pre>

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### CubicBezier-class

### Note

Requires libsbml  $\geq 3.0$ 

# Author(s)

Michael Lawrence

# References

http://sbml.org/documents/

CubicBezier-class SBML type "CubicBezier"

# 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</pre>

### Author(s)

Michael Lawrence

# References

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

Curve-class

#### SBML type "Curve"

#### 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</pre>

### Author(s)

Michael Lawrence

# References

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

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CVTerm-class

# 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"): sets the biologicalQualifierType
   slot.</pre>

modelQualifierType signature(object = "CVTerm"): gets the modelQualifierType slot.

modelQualifierType<- signature(object = "CVTerm"): sets the modelQualifierType slot.</pre>

qualifierType signature(object = "CVTerm"): gets the qualifierType slot.

qualifierType<- signature(object = "CVTerm"): sets the qualifierType slot.</pre>

resources signature(object = "CVTerm"): gets the resources slot.

**resources**<- signature(object = "CVTerm"): sets the resources slot.

### Author(s)

Michael Lawrence

# References

Delay-class

# 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.</pre>

# Note

Requires libsbml >= 3.0

# Author(s)

Michael Lawrence

### References

http://sbml.org/documents/

### See Also

Event

describe

### Description

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", ...).

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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</pre>

### Author(s)

Michael Lawrence

# References

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

Event-class

SBML type "Event"

# Description

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

# Instantiation

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

#### Event-class

# 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 trigger signature(object = "Event"): sets the trigger slot

# Author(s)

Michael Lawrence

#### References

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</pre>

# Author(s)

Michael Lawrence

### References

Experiment-class Experiment

# 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

design signature(object = "Experiment"): Gets the design slot. design<- signature(object = "Experiment"): Sets the design slot. protocol signature(object = "Experiment"): Gets the protocol slot. protocol<- signature(object = "Experiment"): Sets the protocol slot. result signature(object = "Experiment"): Gets the result slot. result<- signature(object = "Experiment"): Sets the result slot. subject signature(object = "Experiment"): Gets the result slot. subject signature(object = "Experiment"): Sets the subject slot.

### Author(s)

Michael Lawrence

# See Also

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</pre>

### Author(s)

Michael Lawrence

#### References

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</pre>

### 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.</pre>

```
symbol signature(object = "InitialAssignment"): gets the symbol slot.
```

symbol<- signature(object = "InitialAssignment"): sets the symbol slot.</pre>

# Note

Requires libsbml >= 3.0

# Author(s)

Michael Lawrence

### References

#### 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

### Author(s)

Michael Lawrence

### References

http://sbml.org/documents/

Layout-class 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" specifing 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.

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#### LineSegment-class

### Methods

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

id<- signature(object = "Layout"): sets the id slot</pre>

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

# 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</pre>
```

# Author(s)

Michael Lawrence

### References

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

math

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) coth(x) coth(x) csch(x) sec(x) sec(x)

### Arguments

The numeric value(s) for the trigonometry operation

#### Model-class

### Value

A numeric vector, the same length as x.

### Author(s)

Michael Lawrence

Model-class

### 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.

SBML type "Model"

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 Speciess. 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.
- constraints: Object of class "list" containing Constraints. The names of the list correspond to the IDs of the elements.

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</pre> name signature(object = "Model"): gets the name slot name<- signature(object = "Model"): sets the name slot</pre> **compartments** signature(object = "Model"): gets the compartments slot compartments<- signature(object = "Model"): sets the compartments slot</pre> events signature(object = "Model"): gets the events slot events<- signature(object = "Model"): sets the events slot</pre> functionDefinitions signature(object = "Model"): gets the functionDefinitions slot functionDefinitions<- signature(object = "Model"): sets the functionDefinitions slot</pre> layouts signature(object = "Model"): gets the layouts slot layouts<- signature(object = "Model"): sets the layouts slot</pre> parameters signature(object = "Model"): gets the parameters slot parameters<- signature(object = "Model"): sets the parameters slot</pre> **species** signature(object = "Model"): gets the species slot species<- signature(object = "Model"): sets the species slot</pre> **reactions** signature(object = "Model"): gets the reactions slot reactions<- signature(object = "Model"): sets the reactions slot</pre> rules signature(object = "Model"): gets the rules slot rules<- signature(object = "Model"): sets the rules slot</pre> unitDefinitions signature(object = "Model"): gets the unitDefinitions slot unitDefinitions<- signature(object = "Model"): sets the unitDefinitions slot</pre> compartmentTypes signature(object = "Model"): gets the compartmentTypes slot **compartmentTypes-** signature(object = "Model"): sets the compartmentTypes slot constraints signature(object = "Model"): gets the constraints slot

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 speciesTypesslot modelHistory signature(object = "Model"): gets the modelHistory slot stoichiometryMatrix signature(object = "Model"): calculates the stoichiometry matrix of the model

### Author(s)

Michael Lawrence

### References

http://sbml.org/documents/

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"): gets the givenName slot. organization signature(object = "ModelCreator"): gets the givenName<- slot. organization signature(object = "ModelCreator"): gets the organization slot. organization<- signature(object = "ModelCreator"): sets the organization slot.</pre>

### Author(s)

Michael Lawrence

### References

http://sbml.org/documents/

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-DDThh: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-DDThh: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.</pre>
- createdDate<- signature(object = "ModelHistory", value = "POSIXt"): Set the createdDate
   slot with a POSIXt instance, obtained e.g. from Sys.time.</pre>
- creators signature(object = "ModelHistory"): gets the creators slot.
- creators<- signature(object = "ModelHistory"): sets the creators slot.</pre>
- modifiedDate signature(object = "ModelHistory"): get the modifiedDate slot.
- modifiedDate<- signature(object = "ModelHistory", value = "POSIXt"): Set the modifiedDate
   slot with a POSIXt instance, obtained e.g. from Sys.time.</pre>

# Author(s)

Michael Lawrence

### References

http://sbml.org/documents/

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ModifierSpeciesReference-class

SBML type "ModifierSpeciesReference"

# 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

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

### Methods

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

### Author(s)

Michael Lawrence

# References

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 value signature(object = "Parameter"): gets the constant slot value signature(object = "Parameter"): gets the value slot

#### ParameterRule-class

### Author(s)

Michael Lawrence

### References

http://sbml.org/documents/

ParameterRule-class SBML type "ParameterRule"

### 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 variable<- 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</pre>

### 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.

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### 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</pre>

### 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

variable signature(object = "RateRule"): gets the variable slot variable<- signature(object = "RateRule"): sets the variable slot</pre>

# 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).

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#### Extends

Class "SBase", directly.

## Methods

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

## Author(s)

Michael Lawrence

# References

http://sbml.org/documents/

ReactionGlyph-class SBML type "ReactionGlyph"

## Description

A glyph representing a Reaction in the SBML layout.

# Instantiation

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

#### 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</pre>

reaction signature(object = "ReactionGlyph"): gets the reaction slot

reaction<- signature(object = "ReactionGlyph"): sets the reaction slot</pre>

# Author(s)

Michael Lawrence

#### References

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

Rule-class

# 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</pre>

# Author(s)

Michael Lawrence

## References

http://sbml.org/documents/

SBase-class

#### 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 notesslot cvTerms signature(object = "SBase"): gets the cvTerms slot. cvTerms<- signature(object = "SBase"): sets the cvTerms slot. sboTerm signature(object = "SBase"): gets the sboTerm slot.

#### Author(s)

Michael Lawrence

## References

http://sbml.org/documents/

SBML import

# Description

Read an SBML file into R.

# Usage

# 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 perfor- mance deficiencies.

# Value

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

# Author(s)

Michael Lawrence

# Examples

```
# 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)</pre>
```

SBML-class

#### 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 = "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</pre>

- model signature(object = "SBML"): gets the model slot
- model<- signature(object = "SBML"): sets the model slot</pre>
- 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</pre>

# Author(s)

Michael Lawrence

# References

http://sbml.org/documents/

# Examples

```
# 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\\_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 document 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 SOSProtocol. See simulate for more details.

#### Author(s)

Michael Lawrence

# References

http://sbml.org/documents/

#### Examples

```
# Read a document into an R DOM
dom <- rsbml_read(system.file("sbml", "GlycolysisLayout.xml", package
= "rsbml"))
# Convert to a graph
graph <- rsbml_graph(dom)
# Write it out to a file
## Not run: rsbml_write(dom, "my.xml")
# Or convert it to a string of XML
rsbml_xml(dom)
# Read into external libsbml data structure
doc <- rsbml_read(system.file("sbml", "GlycolysisLayout.xml", package
= "rsbml"), dom = FALSE)
# Convert it explicitly to an S4 DOM
dom <- rsbml_dom(doc)</pre>
```

SBMLProblem-class SBMLProblem

# Description

Represents an exception thrown during SBML parsing.

# Details

There are trivial subclasses for fatal errors (SBMLFatal), recoverable errors (SBMLError), 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

fatals: A list of SBMLFatal instances.
errors: A list of SBMLError instances.
warnings: A list of SBMLWarning instances.
infos: A list of SBMLInfo instances.

## Methods

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

#### Author(s)

Michael Lawrence

# See Also

The rsbml\_problems function for obtaining an instance of this class describing any problems encountered during parsing.

SimpleSpeciesReference-class
SBML type "SimpleSpeciesReference"

#### Description

Base class for bindings between a Species and a Reaction.

# Instantiation

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

## 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

Class "SBase", directly.

#### SOSDesign-class

#### 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</pre>

# 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 namespaced 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.

.Data: 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

Class "matrix", from data part. Class "ExperimentDesign", directly. Class "array", by class "matrix", distance 2. Class "structure", by class "matrix", distance 3. Class "vector", by class "matrix", distance 4, with explicit coerce.

## Methods

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

#### Author(s)

Michael Lawrence

## References

See <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> 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 <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

## See Also

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

SOSProtocol-class SOSProtocol

## 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: Sclar "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 <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> 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 SOSResult

# 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.

#### 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 <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

# 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

See <a href="http://www.tbi.univie.ac.at/~raim/odeSolver/">http://www.tbi.univie.ac.at/~raim/odeSolver/</a> for more information on the SBML ODE Solver library.

#### 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).

#### Extends

Class "SBase", directly.

#### Methods

id signature(object = "Species"): gets the id slot id<- signature(object = "Species"): sets the id slot</pre> name signature(object = "Species"): gets the name slot name<- signature(object = "Species"): sets the name slot</pre> boundaryCondition signature(object = "Species"): gets the boundaryCondition slot boundaryCondition<- signature(object = "Species"): sets the boundaryCondition slot</pre> charge signature(object = "Species"): gets the charge slot charge<- signature(object = "Species"): sets the charge slot</pre> compartment signature(object = "Species"): gets the compartment slot compartment<- signature(object = "Species"): sets the compartment slot</pre> **constant** signature(object = "Species"): gets the constant slot constant<- signature(object = "Species"): sets the constant slot</pre> units signature(object = "Species"): gets the constant slot units<- signature(object = "Species"): sets the constant slot</pre> 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</pre> 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</pre> substanceUnits signature(object = "Species"): gets the substanceUnits slot substanceUnits<- signature(object = "Species"): sets the substanceUnits slot</pre>

## Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

SpeciesConcentrationRule-class

SBML type "SpeciesConcentrationRule"

## 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

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

# Methods

species signature(object = "SpeciesConcentrationRule"): gets the species slot
species<- signature(object = "SpeciesConcentrationRule"): sets the species slot</pre>

# Author(s)

Michael Lawrence

# References

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 = "SpeciesGlyph"): sets the species slot</pre>

## Author(s)

Michael Lawrence

#### References

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

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

# 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</pre>

#### Author(s)

Michael Lawrence

#### References

http://sbml.org/documents/

#### SpeciesReferenceGlyph-class

SBML type "SpeciesReferenceGlyph"

## 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 underyling 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</pre>

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

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

glyphCurve signature(expr = "SpeciesReferenceGlyph"): gets the glyphCurve slot

glyphCurve<- signature(object = "SpeciesReferenceGlyph"): sets the glyphCurve slot</pre>

#### 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 signature(object = "SpeciesType"): gets the id slot id<- signature(object = "SpeciesType"): sets the id slot name signature(object = "SpeciesType"): gets the name slot name<- signature(object = "SpeciesType"): sets the name slot</pre>

#### Note

Requires libsbml  $\geq 3.0$ 

# 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</pre>
```

#### 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</pre>
```

## 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.</pre>
```

#### Unit-class

## Note

Requires libsbml  $\geq 3.0$ 

# 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: smultiplier \* 10^scale \* x^exponent + 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

```
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
multiplier<- 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"): sets the unitScale slot
```

# Author(s)

Michael Lawrence

## References

http://sbml.org/documents/

UnitDefinition-class SBML type "UnitDefinition"

#### 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).

# UnitDefinition-class

# Extends

Class "SBase", directly.

# Methods

id signature(object = "UnitDefinition"): gets the id slot id<- signature(object = "UnitDefinition"): sets the id slot name signature(object = "UnitDefinition"): gets the name slot name<- signature(object = "UnitDefinition"): sets the name slot units signature(object = "UnitDefinition"): gets the units slot units<- signature(object = "UnitDefinition"): sets the units slot</pre>

# Author(s)

Michael Lawrence

# References

http://sbml.org/documents/

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