Package ‘rsbml’

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Description Links R to libsbml for SBML parsing, validating output,
provides an S4 SBML DOM, converts SBML to R graph objects.
Optionally links to the SBML ODE Solver Library (SOSLib) for
simulating models.
License Artistic-2.0
URL http://www.sbml.org
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R topics documented:

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AlgebraicRule-class

SBML type "AlgebraicRule"

Description

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

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

http://sbml.org/documents/
Slots

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

type: Object of class "character", deprecated.

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

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

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

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

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

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

Extends

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

Methods

variable signature(object = "AssignmentRule"): gets the variable slot

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

type signature(object = "AssignmentRule"): gets the type slot

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

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", ...).
Compartment-class

Slots

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

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

Author(s)

Michael Lawrence

References

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

SBML type "CompartmentGlyph"

Description

A glyph representing a Compartment.

Instantiation

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

Slots

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

Extends

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

Methods

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

Author(s)

Michael Lawrence

References

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

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

Objects from the Class

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

Slots

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

Extends

Class "SBase", directly.

Methods

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

Note

Requires libsbml >= 3.0

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

See Also

Compartment
**CompartmentVolumeRule-class**

*SBML type "CompartmentVolumeRule"*

**Description**

**Obsolete** way to assign a volume to a **Compartment**.

**Instantiation**

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

**Slots**

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

**Extends**


**Methods**

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

**Author(s)**

Michael Lawrence

**References**

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

Note
Requires libsbml >= 3.0

Author(s)
Michael Lawrence

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

A cubic bezier curve in an SBML layout.

**Instantiation**

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

**Slots**

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

**Extends**

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

**Methods**

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

**Author(s)**

Michael Lawrence

**References**

[http://projects.villa-bosch.de/bcb/sbml](http://projects.villa-bosch.de/bcb/sbml)
Curve-class  \textit{SBML type} "Curve"

\textbf{Description}

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

\textbf{Instantiation}

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

\textbf{Slots}

\texttt{curveSegments}: Object of class "list" containing the \texttt{LineSegments} that compose the curve.

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

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

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

\texttt{cvTerms}: Object of class "list" containing instances of \texttt{CVTerm} associated with this element.

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

\textbf{Extends}

Class "\texttt{SBase}", directly.

\textbf{Methods}

\texttt{curveSegments} signature(object = "Curve"): gets the \texttt{curveSegments} slot

\texttt{curveSegments<-} signature(object = "Curve"): sets the \texttt{curveSegments} slot

\textbf{Author(s)}

Michael Lawrence

\textbf{References}

\url{http://projects.villa-bosch.de/bcb/sbml}
CVTerm-class

SBML Type "CVTerm"

Description

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

Objects from the Class

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

Slots

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

Methods

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

Author(s)

Michael Lawrence

References

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

SBML Type "Delay"

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

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

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

Extends
Class "SBase", directly.

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

Note
Requires libsbml >= 3.0

Author(s)
Michael Lawrence

References
http://sbml.org/documents/

See Also
Event


**describe**                          

---

**Describing objects**

**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

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**Dimensions-class**                          

---

**SBML type "Dimensions"**

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**Description**

Holds the size of an SBML layout object.

**Instantiation**

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

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

Extends
Class "SBase", directly.

Methods

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

Author(s)
Michael Lawrence

References
http://projects.villa-bosch.de/bcb/sbml
**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
- **eventAssignments<-** signature(object = "Event"): sets the eventAssignments slot
- **trigger** signature(object = "Event"): gets the trigger slot
- **trigger<-** signature(object = "Event"): sets the trigger slot

**Author(s)**

Michael Lawrence

**References**

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

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

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

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

Extends
Class "SBase", directly.

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

Author(s)
Michael Lawrence

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

This class is an abstraction for an experiment, e.g. in a simulation. An experiment consists of an 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 subject 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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Description

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

Instantiation

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

Slots

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

SBML Type "InitialAssignment"

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

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

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

Extends
Class "SBase", directly.

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

Note
Requires libsbml >= 3.0

Author(s)
- Michael Lawrence

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

**See Also**

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

**KineticLaw-class**  
*SBML type "KineticLaw"

**Description**

Describes the rate of a Reaction.

**Instantiation**

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

**Slots**

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

**Extends**

Class "SBase", directly.

**Methods**

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

**Author(s)**

Michael Lawrence

**References**

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

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

**Extends**

Class "SBase", directly.
Methods

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

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

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

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

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

Author(s)

Michael Lawrence

References

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

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**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.

dend: Object of class "Point" indicating the end position.

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

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

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

MathML Utilities

Description

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

Usage

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

Arguments

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

Value
A numeric vector, the same length as x.

Author(s)
Michael Lawrence

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

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

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

modelHistory: Object of class `ModellHistory` recording the history of the model.

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

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

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

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

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

**Extends**

Class "SBase", directly.

**Methods**

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

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

name signature(object = "Model"): gets the name slot

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

compartments signature(object = "Model"): gets the compartments slot

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

events signature(object = "Model"): gets the events slot

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

functionDefinitions signature(object = "Model"): gets the functionDefinitions slot

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

layouts signature(object = "Model"): gets the layouts slot

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

parameters signature(object = "Model"): gets the parameters slot

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

species signature(object = "Model"): gets the species slot

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

reactions signature(object = "Model"): gets the reactions slot

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

rules signature(object = "Model"): gets the rules slot

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

unitDefinitions signature(object = "Model"): gets the unitDefinitions slot

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

compartmentTypes signature(object = "Model"): gets the compartmentTypes slot

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

constraints signature(object = "Model"): gets the constraints slot
ModelCreator-class

constraints<- signature(object = "Model"): sets the constraints slot
initialAssignments signature(object = "Model"): gets the initialAssignments slot
initialAssignments<- signature(object = "Model"): sets the initialAssignments slot
speciesTypes signature(object = "Model"): gets the speciesTypes slot
speciesTypes<- signature(object = "Model"): sets the speciesTypes slot
modelHistory signature(object = "Model"): gets the modelHistory slot
modelHistory<- signature(object = "Model"): sets the modelHistory slot
stoichiometryMatrix signature(object = "Model"): calculates the stoichiometry matrix of the model

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

ModelCreator-class  SBML Type "ModelCreator"

Description

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

Objects from the Class

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

Slots

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

Methods

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

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ModelHistory-class  SBML Type "ModelHistory"

Description

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

Objects from the Class

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

Slots

createdDate: Object of class "character" representing the date/time of creation, in W3CDTF format: YYYY-MM-DDTh:mm:ssTZD, e.g. "1997-07-16T19:20:30+01:00".

modifiedDate: Object of class "character" representing the date/time of last modification, in W3CDTF format: YYYY-MM-DDTh:mm:ssTZD, e.g. "1997-07-16T19:20:30+01:00".

creators: Object of class "list" of instances of `ModelCreator`, one for each creator of the model.

Methods

createdDate signature(object = "ModelHistory"): get the `createdDate` slot.

createdDate<- signature(object = "ModelHistory", value = "character"): Set the `createdDate` slot to a correctly formatted string.

createdDate<- signature(object = "ModelHistory", value = POSIXt"): Set the `createdDate` slot with a POSIXt instance, obtained e.g. from `Sys.time`.

creators signature(object = "ModelHistory"): gets the `creators` slot.

creators<- signature(object = "ModelHistory"): sets the `creators` slot.

modifiedDate signature(object = "ModelHistory"): get the `modifiedDate` slot.

modifiedDate<- signature(object = "ModelHistory", value = "character"): Set the `modifiedDate` slot to a correctly formatted string.

modifiedDate<- signature(object = "ModelHistory", value = POSIXt"): Set the `modifiedDate` slot with a POSIXt instance, obtained e.g. from `Sys.time`.

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
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


Methods

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

Author(s)

Michael Lawrence

References

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

SBML type "Parameter"

Description

Declares a variable to be used in a mathematical expression.

Instantiation

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

Slots

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

Extends

Class "SBase", directly.

Methods

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

Author(s)
Michael Lawrence

References
http://sbml.org/documents/

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

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

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**Point-class**  
*SBML type "Point"*

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**Description**

Specifies a position in 3D space.

**Instantiation**

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

**Slots**

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

**Extends**

Class "SBase", directly.
RateRule-class

Methods

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

Author(s)

Michael Lawrence

References

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

RateRule-class

SBML type "RateRule"

Description

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

Instantiation

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

Slots

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

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

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

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

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

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

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

Extends

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

**variable** signature(object = "RateRule"): gets the variable slot

**variable<-** signature(object = "RateRule"): sets the variable slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

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### 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).
**ReactionGlyph-class**

**Extends**

Class "SBase", directly.

**Methods**

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

**Author(s)**

Michael Lawrence

**References**

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

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

Author(s)

Michael Lawrence

References

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

SBML type "Rule"

Description

A mathematical equation.

Instantiation

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

Slots

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

**SBML type** "SBase"

---

**Description**

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

**Instantiation**

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

**Slots**

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

**Methods**

- **annotation** signature(object = "SBase"): gets the annotation slot
- **annotation<-** signature(object = "SBase"): sets the annotation slot
- **metaId** signature(object = "SBase"): gets the metaId slot
- **metaId<-** signature(object = "SBase"): sets the metaId slot
- **notes** signature(object = "SBase"): gets the notes slot
- **notes<-** signature(object = "SBase"): sets the notes slot
- **cvTerms** signature(object = "SBase"): gets the cvTerms slot.
- **cvTerms<-** signature(object = "SBase"): sets the cvTerms slot.
- **sboTerm** signature(object = "SBase"): gets the sboTerm slot.
- **sboTerm<-** signature(object = "SBase"): sets the sboTerm slot.

**Author(s)**

Michael Lawrence

**References**

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

Read in an SBML file (start here)

Description

Read an SBML file into R.

Usage

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

Arguments

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

Value

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

Author(s)

Michael Lawrence

Examples

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

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

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

Instantiation

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

Slots

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

Extends

Class "SBase", directly.

Methods

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

- **rsbml_graph** signature(object = "SBML"): converts this document to a graph object.
- **rsbml_check** signature(object = "SBML"): perform consistency checks, see `rsbml_check`.
- **simulate** signature(object = "SBML"): converts this document to an internal `SBMLDocument` and calls `simulate` on it.
- **ver** signature(object = "SBML"): gets the ver slot
- **ver<-** signature(object = "SBML"): sets the ver slot

**Author(s)**

Michael Lawrence

**References**

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

**Examples**

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

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

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

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

---

**SBMLDocument-class**

"SBMLDocument" from libsbml

**Description**

Low-level libsbml document structure.

**Instantiation**

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

**Extends**

Class "oldClass", directly.
Methods

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

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

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

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

rsbml\_write signature(object = "SBMLDocument"): writes this problems encountered during parsing and/or validation.

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)
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

 Thường 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

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.
Slots

- **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


Methods

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

Author(s)

Michael Lawrence

References


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 SOSPprotocol 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 `SOSPprotocol`, 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 `SOSSsubject`, containing the `Model` to be simulated.
- `result`: Object of class `SOSResult` containing the result of the simulation.

**Extends**

Class `Experiment`, directly.

**Methods**

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

**Author(s)**

Michael Lawrence

**References**


**See Also**

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

**Description**

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

**Details**

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

**Objects from the Class**

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

**Slots**

times: A "numeric" vector indicating the time points at which to evaluate the model. Defaults to `tail(seq(0, by = timeStep, length.out = nsim + 1), -1)`. The model is always evaluated at t = 0. This slot is ignored when `indefinite` (below) is TRUE.

timeStep: A scalar "numeric" value, giving the length in time between model evaluations. This is used when calculating the default value of `times`, above, but is otherwise only relevant when the `indefinite` slot, below, is TRUE. Defaults to 1.

indefinite: A scalar "logical", indicating whether the simulation should run indefinitely, i.e. until one of the stopping conditions is met. See `haltOnEvent` and `haltOnSteadyState` below. Defaults to FALSE.

atol: Scalar "numeric", the absolute tolerance in integration error. Defaults to 1e-18.

rtol: Scalar "numeric", the relative tolerance in integration error. Defaults to 1e-10.

maxStep: Scalar "numeric", the maximum number of steps for integration. Not to be confused with `timeStep`, etc, above, which control the simulation time points. Defaults to 10000.

odeMethod: Scalar "character" naming the method for solving ODEs. Either "bdf" (the default) or "adams-moulton".

iterMethod: Scalar "character", naming the iteration method used by the ODE solver, either "newton" (the default) or "functional".

maxOrder: Scalar "numeric" indicating maximum order for the ODE solver. Defaults to 5.

sensMethod: Scalar "character" naming the method for sensitivity analysis. One of "none" (the default and currently the only valid option), "simultaneous", "staggered" or "staggered1".

haltOnEvent: Scalar "logical" indicating whether the simulation should halt when the model emits an Event. This allows the model to stop the simulation when some state is reached. Defaults to FALSE.

haltOnSteadyState: Scalar "logical", indicating whether to halt when a steady state is detected. Defaults to FALSE.

useJacobian: Scalar "logical" indicating whether to use Jacobian ASTs (TRUE, the default) or the internal approximation in the CVODES library.

storeResults: Scalar "logical" indicating whether to store the entire time course (TRUE, the default) or just the last time point. Just for performance.
SOSResult-class

Extends

Class "ExperimentProtocol", directly.

Methods

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

Author(s)

Michael Lawrence

References


See Also

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

SOSResult-class

<table>
<thead>
<tr>
<th>SOSResult-class</th>
<th>SOSResult</th>
</tr>
</thead>
</table>

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 \texttt{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 Compartments 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 \url{http://www.tbi.univie.ac.at/~raim/odeSolver/} for more information on the SBML ODE Solver library.

See Also

\texttt{SOSExperiment} for running a simulation and obtaining an instance of this class.
Species-class

See Also

SOSExperiment for running a simulation on a SOSSubject.

Species-class SBML type "Species"

Description

A participant in an SBML model.

Instantiation

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

Slots

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

name: Object of class "character" naming this component.

compartment: Object of class "character" identifying the compartment in which this species is located.

initialAmount: Object of class "numeric" indicating the initial amount for this species (mutually exclusive with initialConcentration).

initialConcentration: Object of class "numeric" indicating the initial concentration for this species (mutually exclusive with initialAmount).

substanceUnits: Object of class "character" identifying the units for the amount of this species or the numerator of the concentration.

spatialSizeUnits: Object of class "character" identifying the units for the denominator of the species concentration.

hasOnlySubstanceUnits: Object of class "logical" indicating whether the quantity of this species is specified as an amount or a concentration.

boundaryCondition: Object of class "logical". If TRUE, indicates that the quantity of this species cannot be changed by a reaction.

charge: Object of class "integer" indicating the electrical charge of this species.

constant: Object of class "logical" indicating whether the quantity of this species can change.

units: Object of class "character", deprecated.

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

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

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

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

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
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


Methods

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

Author(s)

Michael Lawrence

References

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

**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


Methods

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
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 underlying *SpeciesReference*.
- `speciesReference`: Object of class "character" identifying the link of a *SpeciesReference* represented by this glyph.
- `role`: Object of class "character" indicating how this glyph should represent the "role" of the underlying *SpeciesReference*.
- `glyphCurve`: Object of class "Curve" describing this glyph as a curve (optional).
- `id`: Object of class "character" uniquely identifying this component.
- `boundingBox`: Object of class "BoundingBox" describing the position and size of the graphical object.
- `metaId`: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- `notes`: Object of class "character" containing user-readable XHTML notes about an element.
- `annotation`: Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- `cvTerms`: Object of class "list" containing instances of CVTerm associated with this element.
- `sboTerm`: Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

**Extends**

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

**Methods**

- `role` signature(object = "SpeciesReferenceGlyph"): gets the role slot
- `role<-` signature(object = "SpeciesReferenceGlyph"): sets the role slot
- `speciesGlyph` signature(object = "SpeciesReferenceGlyph"): gets the speciesGlyph slot
- `speciesGlyph<-` signature(object = "SpeciesReferenceGlyph"): sets the speciesGlyph slot
- `speciesReference` signature(object = "SpeciesReferenceGlyph"): gets the speciesReference slot
SpeciesType-class

**speciesReference**<- signature(object = "SpeciesReference Glyph"): sets the speciesReference slot

**glyphCurve** signature(expr = "SpeciesReference Glyph"): gets the glyphCurve slot

**glyphCurve**<- signature(object = "SpeciesReference Glyph"): sets the glyphCurve slot

Author(s)

Michael Lawrence

References

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

---

**SpeciesType-class**

**SBML Type** "SpeciesType"

---

**Description**

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

**Objects from the Class**

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

**Slots**

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

name: Object of class "character" naming this component.

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

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

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

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

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

**Extends**

Class "SBase", directly.

**Methods**

**id** 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
Note
Requires libsbml >= 3.0

Author(s)
Michael Lawrence

References
http://sbml.org/documents/

See Also
Species

---

**StoichiometryMath-class**

*SBML type* "StoichiometryMath"

---

**Description**

Dynamically defines the stoichiometry of a `SpeciesReference`.

**Instantiation**

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

**Slots**

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

**Extends**

Class "SBase", directly.

**Methods**

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

Author(s)
Michael Lawrence

References
http://sbml.org/documents/

---

TextGlyph-class  SBML type "TextGlyph"

Description
A run of text in an SBML layout.

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

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

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

graphicalObject signature(object = "TextGlyph"): gets the graphicalObject slot

graphicalObject<- signature(object = "TextGlyph"): sets the graphicalObject slot

originOfText signature(object = "TextGlyph"): gets the originOfText slot

originOfText<- signature(object = "Text Glyph"): sets the originOfText slot

text signature(x = "TextGlyph"): ...

text<- signature(object = "TextGlyph"): sets the text slot

Author(s)

Michael Lawrence

References

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

Trigger-class

SBML Type ”Trigger”

Description

Expresses when an Event should be fired.

Objects from the Class

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

Slots

math: Object of class "expression" that evaluates to TRUE when the event should be fired.

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

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

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

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

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

Extends

Class "SBase", directly.

Methods

math signature(domain = "Trigger"): gets the math slot.

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

### Note

Requires libsbml >= 3.0

### Author(s)

Michael Lawrence

### References

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

### See Also

- [Event](#), the parent of this element.

---

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

### Description

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

### Instantiation

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

### Slots

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

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

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

\begin{verbatim}
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).
\end{verbatim}
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

Author(s)

Michael Lawrence

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http://sbml.org/documents/
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