Package ‘rsbml’
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Title  R support for SBML, using libsbml
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Imports  BiocGenerics, graph, utils
SystemRequirements  libsbml (==5.10.2)
Maintainer  Michael Lawrence <michafla@gene.com>
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
biocViews  GraphAndNetwork, Pathways, Network
NeedsCompilation  yes

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 "SBBase", by class "Rule", distance 2.

Methods

- No methods defined with class "AlgebraicRule" in the signature.

Author(s)

- Michael Lawrence

References

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

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

Description

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

Instantiation

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

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

Extends

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

Methods

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

**Description**

Species the size and position of an SBML layout object.

**Instantiation**

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

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

Compartment-class

SBML type "Compartment"

Description

A bounded space that contains Species.

Instantiation

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

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/
**Description**

A glyph representing a *Compartment*.

**Instantiation**

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

**Slots**

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

**Extends**

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

**Methods**

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

**Author(s)**

Michael Lawrence 

**References**

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

SBML Type "CompartmentType"

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

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

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

Extends
Class "SBase", directly.

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

Note
Requires libsbml >= 3.0

Author(s)
Michael Lawrence

References
http://sbml.org/documents/

See Also
Compartment
CompartmentVolumeRule-class

SBML type "CompartmentVolumeRule"

Description

Obsolete way to assign a volume to a Compartment.

Instantiation

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

Slots

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

Extends


Methods

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

Author(s)

Michael Lawrence

References

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

SBML Type "Constraint"

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

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

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

Extends
Class "SBase", directly.

Methods
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/
CubicBezier-class

SBML type "CubicBezier"

Description
A cubic bezier curve in an SBML layout.

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

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

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

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

Author(s)
Michael Lawrence

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

SBML type "Curve"

Description

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

Instantiation

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

Slots

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

Description

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

Objects from the Class

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

Slots

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

Methods

- `biologicalQualifierType` signature(object = "CVTerm"): 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**

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"

**Description**

Holds the size of an SBML layout object.

**Instantiation**

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

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

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**Event-class**

**SBML type"Event"**

**Description**

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

**Instantiation**

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

**Experiment**

**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/
GraphicalObject-class  SBML type "GraphicalObject"

Description

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

Instantiation

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

Slots

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

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

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

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

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

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

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

Extends

Class "SBase", directly.

Methods

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

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

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

Author(s)

Michael Lawrence

References

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

SBML Type "InitialAssignment"

**Description**

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

**Objects from the Class**

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

**Slots**

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

**Extends**

Class "SBase", directly.

**Methods**

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

**Note**

Requires libsbml >= 3.0

**Author(s)**

Michael Lawrence

**References**

http://sbml.org/documents/
See Also

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

---

KineticLaw-class  

**SBML type** "KineticLaw"

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**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

SBML type "Layout"

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

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

Slots

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

Extends
Class "SBase", directly.
Methods

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

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

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

Author(s)

Michael Lawrence

References

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

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

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

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

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

Extends

Class "SBase", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

MathML Utilities

Description

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

Usage

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

Arguments

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

Value

A numeric vector, the same length as x.

Author(s)

Michael Lawrence

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Model-class  
SBML type "Model"

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.
- `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
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

Description

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

Objects from the Class

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

Slots

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

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

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

Methods

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/
Description

Identifies a Species that modifies the parent Reaction.

Instantiation

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

Slots

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

Extends

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

Methods

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

Author(s)

Michael Lawrence

References

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
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"

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

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**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.
Reaction-class

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/

---

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/)

---

**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/
**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/
SBML import

Read an SBML file into R.

Usage

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

Arguments

filename    the name of the SBML file to parse

text        a string of SBML text to parse (instead of file)

dom         whether to convert directly to the S4 DOM (TRUE, the default) or leave as the internal SBMLDocument.

strict      whether to report warnings in addition to errors or not (FALSE, the default).

schema      whether to perform XML schema validation

consistency whether to perform consistency checks; recommended but might cause performance deficiencies.

Value

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

Author(s)

Michael Lawrence

Examples

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

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

SBML type "SBML"

Description

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

Instantiation

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

Slots

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

Extends

Class "SBase", directly.

Methods

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

Low-level libsbml document structure.

**Instantiation**

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

**Extends**

Class "oldClass", directly.

---

**rsbml_graph** signature(object = "SBML"): converts this document to a graph object.

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

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

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

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

**Author(s)**

Michael Lawrence

**References**

http://sbml.org/documents/

**Examples**

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

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

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

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

rsbml\_check signature(object = "SBMLDocument"): rsbml\_check(object, strict = FALSE, consistency = TRUE): 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 document to a file as SBML.

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

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

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

Examples

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

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

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

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

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

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

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

Description

A class representing errors encountered during parsing of SBML.

Slots

- `fatalis`: A list of SBMLFatal instances.
- `errors`: A list of SBMLError instances.
- `warnings`: A list of SBMLWarning instances.
- `infos`: A list of SBMLInfo instances.
Methods

- **.throw** signature(object = "SBMLProblems"): Throws each SBMLProblem in this object.
- **errors** signature(object = "SBMLProblems"): Gets the errors slot.
- **fatalss** 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.
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

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

See Also

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

SOSExperiment-class  SOS Experiment

Description

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

Details

The general workflow for running a simulation:

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

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

**Objects from the Class**

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

**Slots**

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

**Extends**

Class `Experiment`, directly.

**Methods**

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

**Author(s)**

Michael Lawrence

**References**


**See Also**

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

Description

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

Details

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

Objects from the Class

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

Slots

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Extends

Class "ExperimentProtocol", directly.

Methods

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

Author(s)

Michael Lawrence

References

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

See Also

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

SOSResult-class  SOSResult

Description

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

Slots

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

  sample  A factor, the run number, only exists if there were multiple runs, see SOSDesign.
  type  A factor, the SBML element type for the time course, e.g. "species".
  id  A factor, the id of the SBML element for the time course.
  time  The numeric time value for the time point.
  value  The actual numeric value for the time course at that time.

sens: A "matrix" with results from sensitivity analysis, not yet supported.

Extends

Class "ExperimentResult", directly.
Methods

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

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

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

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

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

Author(s)

Michael Lawrence

References

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

See Also

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

SOSSubject-class   SOSSubject

Description

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

Objects from the Class

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

Extends

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

Author(s)

Michael Lawrence

References

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

SBML type "Species"

See Also

SOSExperiment for running a simulation on a SOSSubject.

Species-class

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/]
SpeciesGlyph-class  SBML type "SpeciesGlyph"

Description

A glyph representing a Species in an SBML layout.

Instantiation

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

Slots

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

Extends

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

Methods

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

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 `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

SpeciesType<- signature(object = "SpeciesReferenceGlyph"): sets the speciesReference slot
glyphCurve signature(expr = "SpeciesReferenceGlyph"): gets the glyphCurve slot
glyphCurve<- signature(object = "SpeciesReferenceGlyph"): sets the glyphCurve slot

Author(s)

Michael Lawrence

References

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

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

\textit{SBML} type "StoichiometryMath"

Description
Dynamically defines the stoichiometry of a \textit{SpeciesReference}.

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

Slots

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

Extends
Class "SBase", directly.

Methods

\texttt{math signature(object = "StoichiometryMath"): gets the math slot}
\texttt{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.
Trigger-class

Methods

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

Author(s)

Michael Lawrence

References

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

---

**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.
Note

Requires libsbml >= 3.0

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

See Also

Event, the parent of this element.

Unit-class

\textit{SBML type} "Unit"

Description

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

Instantiation

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

Slots

\texttt{kind}: Object of class "character" identifying a SBML \textit{UnitKind}. For possible values see Table 2 in the SBML specification.

\texttt{exponent}: Object of class "integer" indicating the exponent to use in the transformation.

\texttt{unitScale}: Object of class "integer" indicating the order of magnitude of the scaling to use in the transformation.

\texttt{multiplier}: Object of class "numeric" indicating the factor to use for scaling in the transformation.

\texttt{offset}: Object of class "numeric" indicating the amount of constant shift in the transformation.

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

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

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

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

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

Class "SBase", directly.

Methods

- **exponent** signature(object = "Unit"): gets the exponent slot
- **exponent<-** signature(object = "Unit"): sets the exponent slot
- **kind** signature(object = "Unit"): gets the kind slot
- **kind<-** signature(object = "Unit"): sets the kind slot
- **multiplier** signature(object = "Unit"): gets the multiplier slot
- **multiplier<-** signature(object = "Unit"): sets the multiplier slot
- **offset** signature(object = "Unit"): gets the offset slot
- **offset<-** signature(object = "Unit"): sets the offset slot
- **unitScale** signature(x = "Unit"): ... 
- **unitScale<-** signature(object = "Unit"): sets the unitScale slot

Author(s)

Michael Lawrence

References

http://sbml.org/documents/

---

**UnitDefinition-class**  
*SBML type "UnitDefinition"*

**Description**

Associates one or more *Units* with an ID and name.

**Instantiation**

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

**Slots**

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

References

http://sbml.org/documents/
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