

Package: rsbml (via r-universe)

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Title R support for SBML, using libsbml

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Imports BiocGenerics, graph, utils

SystemRequirements libsbml (==5.10.2)

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

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URL <http://www.sbml.org>

biocViews GraphAndNetwork, Pathways, Network

Repository <https://bioc.r-universe.dev>

RemoteUrl <https://github.com/bioc/rsbml>

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AlgebraicRule-class *SBML type "AlgebraicRule"*

Description

Expresses equations that are not assignments nor rates of change.

Instantiation

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

Slots

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

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[Rule](#)", directly. Class "[SBase](#)", by class "Rule", distance 2.

Methods

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

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/>

| | |
|-------------------|--------------------------------|
| BoundingBox-class | <i>SBML type "BoundingBox"</i> |
|-------------------|--------------------------------|

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", ...)`.

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/>

CompartementGlyph-class

SBML type "CompartementGlyph"

Description

A glyph representing a [Compartment](#).

Instantiation

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

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>

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

Class "[AssignmentRule](#)", directly. Class "[Rule](#)", by class "AssignmentRule", distance 2. Class "[SBase](#)", by class "AssignmentRule", distance 3.

Methods

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

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

| | |
|------------------|-------------------------------|
| Constraint-class | <i>SBML Type "Constraint"</i> |
|------------------|-------------------------------|

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 | <i>SBML type "CubicBezier"</i> |
|-------------------|--------------------------------|

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

*SBML Type "CVTerm"***Description**

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

Objects from the Class

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

Slots

qualifierType: Object of class "character" specifying the type of qualifier for this term. Types "model" and "biological" have special meaning, but any string may be specified.

modelQualifierType: Object of class "character" specifying the type of model qualifier, if **qualifierType** is set to "model". Types "is" and "isDescribedBy" are formally defined in MIRIAM, but any string may be specified.

biologicalQualifierType: Object of class "character" specifying the type of biological qualifier, if **qualifierType** is set to "biological". Types "is", "hasPart", "isPartOf", "isVersionOf", "hasVersion", "isHomologTo", and "isDescribedBy" are formally defined in MIRIAM, though any string may be specified.

resources: Object of class "character" specifying a URI that identifies some resource related an SBML element by the qualifier.

Methods

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

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

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

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

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

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

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

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

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 | <i>Describing objects</i> |
|----------|---------------------------|

Description

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

Usage

```
describe(object, ...)
```

Arguments

| | |
|---------------------|-----------------------------------|
| <code>object</code> | The object to be described. |
| <code>...</code> | Additional arguments for methods. |

Value

A short textual (string) representation of object.

Describable objects

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

Describable methods

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

Author(s)

Michael Lawrence

| | |
|------------------|-------------------------------|
| Dimensions-class | <i>SBML type "Dimensions"</i> |
|------------------|-------------------------------|

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>

 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 | <i>Experiment</i> |
|------------------|-------------------|

Description

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

Objects from the Class

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

Slots

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

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

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

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

Methods

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

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

Layout-class

SBML type "Layout"

Description

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

Instantiation

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

Slots

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

Extends

Class "[SBase](#)", directly.

Methods

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

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

Author(s)

Michael Lawrence

References

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

LineSegment-class *SBML type "LineSegment"*

Description

Describes a simple A-B line.

Instantiation

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

Slots

start: Object of class "Point" indicating the start position.

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

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[SBBase](#)", 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>

math

MathML Utilities

Description

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

Usage

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

Arguments

x The numeric value(s) for the trigonometry operation

Value

A numeric vector, the same length as x.

Author(s)

Michael Lawrence

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.

layouts: Object of class "list" containing [Layouts](#). The names of the list correspond to the IDs of the elements.

speciesTypes: Object of class "list" containing [SpeciesTypes](#). The names of the list correspond to the IDs of the elements.

compartmentTypes: Object of class "list" containing [CompartmentTypes](#). The names of the list correspond to the IDs of the elements.

constraints: Object of class "list" containing [Constraints](#). The names of the list correspond to the IDs of the elements.

initialAssignments: Object of class "list" containing [InitialAssignments](#).

modelHistory: Object of class [ModelHistory](#) recording the history of the model.

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[SBase](#)", directly.

Methods

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

constraints signature(object = "Model"): gets the constraints slot
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.

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

ModelHistory-class *SBML Type "ModelHistory"*

Description

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

Objects from the Class

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

Slots

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

Methods

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

ModifierSpeciesReference-class
SBML type "ModifierSpeciesReference"

Description

Identifies a [Species](#) that modifies the parent [Reaction](#).

Instantiation

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

Slots

- id:** Object of class "character" uniquely identifying this component.
- species:** Object of class "character" identifying the [Species](#) being referenced.
- metaId:** Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- notes:** Object of class "character" containing user-readable XHTML notes about an element.

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

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 | <i>SBML type "Parameter"</i> |
|-----------------|------------------------------|

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

Class "[AssignmentRule](#)", directly. Class "[Rule](#)", by class "AssignmentRule", distance 2. Class "[SBase](#)", by class "AssignmentRule", distance 3.

Methods

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

Point-class

SBML type "Point"

Description

Specifies a position in 3D space.

Instantiation

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

Slots

x: Object of class "numeric" indicating the X coordinate

y: Object of class "numeric" indicating the Y coordinate

z: Object of class "numeric" indicating the Z coordinate

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[SBase](#)", directly.

Methods

x signature(object = "Point"): gets the x slot

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

y signature(object = "Point"): gets the y slot

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

z signature(object = "Point"): gets the z slot

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

Author(s)

Michael Lawrence

References

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

| | |
|----------------|----------------------|
| RateRule-class | SBML type "RateRule" |
|----------------|----------------------|

Description

An equation that describes the rate of change in the quantity of a [Species](#), the size of a [Compartment](#) or the value of a [Parameter](#).

Instantiation

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

Slots

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

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

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[Rule](#)", directly. Class "[SBase](#)", by class "Rule", distance 2.

Methods

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

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

| | |
|----------------|-----------------------------|
| Reaction-class | <i>SBML type "Reaction"</i> |
|----------------|-----------------------------|

Description

Any transformation, transportation or binding process that changes the quantity of one or more [Species](#).

Instantiation

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

Slots

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

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

reactants: Object of class "list" containing [SpeciesReferences](#) specifying the [Species](#) that are reactants for this reaction. The names of the list correspond to the IDs of the species.

products: Object of class "list" containing [SpeciesReferences](#) specifying the [Species](#) that are products for this reaction. The names of the list correspond to the IDs of the species.

modifiers: Object of class "list" containing [ModifierSpeciesReferences](#) specifying the [Species](#) that are modifiers for this reaction. The names of the list correspond to the IDs of the species.

kineticLaw: Object of class "KineticLaw" that dynamically defines the rate of the reaction.

reversible: Object of class "logical" indicating whether the direction of this reaction is reversible.

fast: Object of class "logical" indicating whether this reaction should be considered instantaneous relative to non-fast reactions.

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[SBase](#)", directly.

Methods

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

ReactionGlyph-class *SBML type "ReactionGlyph"*

Description

A glyph representing a [Reaction](#) in the SBML layout.

Instantiation

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

Slots

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

Extends

Class "[GraphicalObject](#)", directly. Class "[SBase](#)", by class "[GraphicalObject](#)", distance 2.

Methods

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

Author(s)

Michael Lawrence

References

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

| | |
|------------|-------------------------|
| Rule-class | <i>SBML type "Rule"</i> |
|------------|-------------------------|

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 notesslot

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

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

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

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

SBML import

Read in an SBML file (start here)

Description

Read an SBML file into R.

Usage

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

Arguments

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

Value

a [SBML](#) object, or a [SBMLDocument](#) if dom is FALSE.

Author(s)

Michael Lawrence

Examples

```
# 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 "[SBBase](#)", directly.

Methods

coerce signature(from = "SBMLDocument", to = "SBML"): constructs the S4 object model from a low-level libsbml document.

coerce signature(from = "SBML", to = "SBMLDocument"): converts the S4 object model to a low-level libsbml document.

coerce signature(from = "SBML", to = "graph"): converts the S4 object model to a graph.

level signature(object = "SBML"): gets the level slot

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

model signature(object = "SBML"): gets the model slot

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

rsbml\doc signature(model = "SBML"): converts the S4 object model to a low-level libsbml document.

rsbml\write signature(object = "SBML"): writes this document to a file as SBML.

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

rsbml\graph signature(object = "SBML"): converts this document to a graph object.

rsbml\check signature(object = "SBML"): perform consistency checks, see [rsbml_check](#).

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

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

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

Examples

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

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

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

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

SBMLDocument-class *"SBMLDocument" from libsbml*

Description

Low-level libsbml document structure.

Instantiation

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

Extends

Class "[oldClass](#)", directly.

Methods

rsbml_check signature(object = "SBMLDocument"): `rsbml_check(object, strict = FALSE, consistency = 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 | <i>SBMLProblem</i> |
|-------------------|--------------------|

Description

Represents an exception thrown during SBML parsing.

Details

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

Slots

line: The "numeric" line number in the SBML file where the problem was detected.

column: Object of class "numeric" column number in the SBML file where the problem was detected.

msg: Object of class "character", a human-readable description of the problem.

Methods

.condition signature(object = "SBMLProblem"): constructs a [condition](#) object representing the exception.

Author(s)

Michael Lawrence

See Also

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

SBMLProblems-class *SBMLProblems*

Description

A class representing errors encountered during parsing of SBML.

Slots

fatals: A list of [SBMLFatal](#) instances.

errors: A list of [SBMLError](#) instances.

warnings: A list of [SBMLWarning](#) instances.

infos: A list of [SBMLInfo](#) instances.

Methods

.throw signature(object = "SBMLProblems"): Throws each [SBMLProblem](#) in this object.

errors signature(object = "SBMLProblems"): Gets the errors slot.

fatals signature(object = "SBMLProblems"): Gets the fatals slot.

infos signature(object = "SBMLProblems"): Gets the infos slot.

warns signature(object = "SBMLProblems"): Gets the warns slot.

Author(s)

Michael Lawrence

See Also

The [rsbml_problems](#) function for obtaining an instance of this class describing any problems encountered during parsing.

SimpleSpeciesReference-class
SBML type "SimpleSpeciesReference"

Description

Base class for bindings between a [Species](#) and a [Reaction](#).

Instantiation

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

Slots

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

Extends

Class "[SBase](#)", directly.

Methods

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

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

SOSDesign-class

SOSDesign

Description

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

Details

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

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

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

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

Objects from the Class

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

Slots

`.Data`: Object of class `"matrix"`, holding the parameter settings.

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

Extends

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

Methods

`reactions` signature(object = "SOSDesign"): gets the reactions slot.

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

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

See Also

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

SOSProtocol-class *SOSProtocol*

Description

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

Details

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

Objects from the Class

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

Slots

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

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 | <i>SOSResult</i> |
|-----------------|------------------|

Description

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

Slots

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

sample A factor, the run number, only exists if there were multiple runs, see [SOSDesign](#).

type A factor, the SBML element type for the time course, e.g. "species".

id A factor, the id of the SBML element for the time course.

time The numeric time value for the time point.

value The actual numeric value for the time course at that time.

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

Extends

Class "[ExperimentResult](#)", directly.

Methods

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

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

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

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

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

Author(s)

Michael Lawrence

References

See <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 | <i>SOSSubject</i> |
|------------------|-------------------|

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.

See Also

[SOSExperiment](#) for running a simulation on a SOSSubject.

| | |
|---------------|----------------------------|
| Species-class | <i>SBML type "Species"</i> |
|---------------|----------------------------|

Description

A participant in an SBML model.

Instantiation

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

Slots

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

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

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

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

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

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

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

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

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

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

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

units: Object of class "character", deprecated.

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "SBase", directly.

Methods

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

Class "[AssignmentRule](#)", directly. Class "[Rule](#)", by class "AssignmentRule", distance 2. Class "[SBase](#)", by class "AssignmentRule", distance 3.

Methods

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

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

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

Class "[SimpleSpeciesReference](#)", directly. Class "[SBase](#)", by class "[SimpleSpeciesReference](#)", distance 2.

Methods

stoichiometry signature(object = "SpeciesReference"): gets the stoichiometry slot

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

stoichiometryMath signature(object = "SpeciesReference"): gets the stoichiometryMath slot

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 `linkS4class{SpeciesReference}` represented by this glyph.
- role:** Object of class "character" indicating how this glyph should represent the "role" of the underlying [SpeciesReference](#).
- glyphCurve:** Object of class "Curve" describing this glyph as a curve (optional).
- id:** Object of class "character" uniquely identifying this component.
- boundingBox:** Object of class "BoundingBox" describing the position and size of the graphical object.
- metaId:** Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
- notes:** Object of class "character" containing user-readable XHTML notes about an element.
- annotation:** Object of class "character" containing additional machine-readable information about an element, usually as RDF, such as BioPAX. This is where application-specific data belongs.
- cvTerms:** Object of class "list" containing instances of [CVTerm](#) associated with this element.
- sboTerm:** Object of class "integer" identifying a term in the Systems Biology Ontology (SBO).

Extends

Class "[GraphicalObject](#)", directly. Class "[SBase](#)", by class "[GraphicalObject](#)", distance 2.

Methods

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

SpeciesType-class *SBML Type "SpeciesType"*

Description

A [Species](#) represents a pool of a chemical in a particular `linkS4class{Compartment}`. This element specifies a type of species, that is, the chemical independent of location.

Objects from the Class

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

Slots

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

Extends

Class "[SBase](#)", directly.

Methods

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

Note

Requires libsbml >= 3.0

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

See Also

[Species](#)

StoichiometryMath-class
SBML type "StoichiometryMath"

Description

Dynamically defines the stoichiometry of a [SpeciesReference](#).

Instantiation

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

Slots

math: Object of class "expression" that evaluates to the stoichiometric coefficient.
metaId: Object of class "character" that is an XML ID "described" by an RDF resource. This links an SBML element to an RDF resource. RDF may appear anywhere in an SBML element, but is usually placed inside the annotation element.
notes: Object of class "character" containing user-readable XHTML notes about an element.

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[SBase](#)", directly.

Methods

math signature(object = "StoichiometryMath"): gets the math slot

math<- signature(object = "StoichiometryMath"): sets the math slot

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

| | |
|-----------------|------------------------------|
| TextGlyph-class | <i>SBML type "TextGlyph"</i> |
|-----------------|------------------------------|

Description

A run of text in an SBML layout.

Instantiation

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

Slots

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

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

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

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

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

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[GraphicalObject](#)", directly. Class "[SBase](#)", by class "GraphicalObject", distance 2.

Methods

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

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

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

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

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

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

Author(s)

Michael Lawrence

References

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

Trigger-class

SBML Type "Trigger"

Description

Expresses when an [Event](#) should be fired.

Objects from the Class

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

Slots

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

Extends

Class "[SBase](#)", directly.

Methods

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

Note

Requires `libsbml >= 3.0`

Author(s)

Michael Lawrence

References

<http://sbml.org/documents/>

See Also

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

| | |
|------------|-------------------------|
| Unit-class | <i>SBML type "Unit"</i> |
|------------|-------------------------|

Description

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

Instantiation

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

Slots

kind: Object of class "character" identifying a an SBML UnitKind. For possible values see Table 2 in the SBML specification.

exponent: Object of class "integer" indicating the exponent to use in the transformation.

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

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

offset: Object of class "numeric" indicating the amount of constant shift in the transformation.

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

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

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

cvTerms: Object of class "list" containing instances of [CVTerm](#) associated with this element.

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

Extends

Class "[SBase](#)", directly.

Methods

exponent signature(object = "Unit"): gets the exponent slot

exponent<- signature(object = "Unit"): sets the exponent slot

kind signature(object = "Unit"): gets the kind slot

kind<- signature(object = "Unit"): sets the kind slot

multiplier signature(object = "Unit"): gets the multiplier slot

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