

# Package ‘rsbml’

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**Title** R support for SBML, using libsbml

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**Depends** R (>= 2.6.0), BiocGenerics (>= 0.3.2), methods, utils

**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.

**License** Artistic-2.0

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

**biocViews** GraphAndNetwork, Pathways, Network

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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/>

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BoundingBox-class	SBML type "BoundingBox"
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**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>
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### 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/>

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

### 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

*Describing objects*

---

**Description**

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

**Usage**

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

**Arguments**

<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>
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---

**Description**

Holds the size of an SBML layout object.

**Instantiation**

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

**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/>

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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/>

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Experiment-class	<i>Experiment</i>
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---

**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	<i>SBML type "RateRule"</i>
----------------	-----------------------------

---

### 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 <a href="#">SBMLDocument</a> .
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	<i>SOSProtocol</i>
-------------------	--------------------

---

**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>
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---

## 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.

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SOSSubject-class	<i>SOSSubject</i>
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**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>
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**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>
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---

### 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>
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---

### Description

A (possibly transformed) reference to a base UnitKind. The transformation is of the form: \$multiplier \* 10<sup>scale</sup> \* x<sup>exponent</sup> + 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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