SBMLR

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`Ops.SBML` *Check the equality of the species and reactions of two SBML models*

Description

This function tests the equivalence of two models with respect to the species and reaction data frames generated by summary.

Usage

```
## S3 method for class 'SBML'
Ops(e1,e2)
```

Arguments

`e1`	The first of the two model objects of class SBML which are to be compared.
`e2`	The second model object.

Value

A list containing the following two boolean dataframes

`species`	The equality of species information tabularized as a data frame.
`reactions`	The equality of reaction information tabularized as a dataframe.

Author(s)

Tom Radivoyevitch

See Also

`summary.SBML`

Examples

```
library(SBMLR)
curto1=readSBMLR(file.path(system.file(package="SBMLR"), "models/curto.r"))
curto2=readSBML(file.path(system.file(package="SBMLR"), "models/curto.xml"))
curto1==curto2
```

`readSBML` *Convert an SBML file into an R model object of class SBML*

Description

This function converts an SBML level 2 file into a corresponding R model structure of class `SBML`.

Usage

```
readSBML(filename)
```

Arguments

`filename`	An SBML level 2 model input file.

Details

A limited subset of SBML level 2 models is currently supported, e.g. events and function definitions are not covered.

Value

A corresponding SBML model object in R.

Note

This function replaces `read.SBML` of older versions.

Author(s)

Tom Radivoyevitch

See Also

`readSBMLR`

Examples

```
library(SBMLR)
library(odesolve)
curtoX=readSBML(file.path(system.file(package="SBMLR"), "models/curto.xml"))
curtoR=readSBMLR(file.path(system.file(package="SBMLR"), "models/curto.r"))
curtoX==curtoR
```

`readSBMLR` *Convert an SBMLR file into an R model object of class SBML*

Description

This function converts an SBMLR model definition in filename into a corresponding returned SBML model structure.

Usage

```
readSBMLR(filename)
```

Arguments

`filename`	An SBMLR model definition file.

Details

A limited subset of SBML level 2 models is currently supported, e.g. events and function definitions are not covered.

Value

A corresponding `SBML` model object in R.

Note

This function replaces the use of `source` in older versions of SBMLR. It includes rate law and rule string to function, expression and MathML mappings.

Author(s)

Tom Radivoyevitch

See Also

`readSBML`

Examples

```
library(SBMLR)
library(odesolve)
curtoX=readSBML(file.path(system.file(package="SBMLR"), "models/curto.xml"))
curtoR=readSBMLR(file.path(system.file(package="SBMLR"), "models/curto.r"))
curtoX==curtoR
```

`saveSBML` *Saves an R model object as an SBML file*

Description

This function converts a class `SBML` model object in R into an SBML level 2 file.

Usage

```
saveSBML(model,filename)
```

Arguments

`model`	The model object in R.
`filename`	The name of the SBML file

Details

The output file is SBML level 2.

Value

No value returned.

Warning

SBML events and function definitions are NOT implemented.

Note

For speed, the SBML file is written incrementally, rather than first built as a DOM in R and then saved using `xmlSave`.

Author(s)

Tom Radivoyevitch

References

Radivoyevitch, T. A two-way interface between limited Systems Biology Markup Language and R. BMC Bioinformatics 5, 190 (2004).

See Also

`saveSBMLR`

Examples

```
library(SBMLR)
library(odesolve)
curtoR=readSBMLR(file.path(system.file(package="SBMLR"), "models/curto.r"))
saveSBML(curtoR,"curtoR.xml")
curtoX=readSBML("curtoR.xml")
curtoX==curtoR
summary(curtoR)
unlink("curtoR.xml")
```

---

saveSBMLR *Save an R model object of class SBML as an SBMLR file*

Description

This function converts SBML model object in R into an SBMLR model definition file.

Usage

```
saveSBMLR(model,filename)
```

Arguments

model	The SBML model object to be mapped into the SBMLR model definition file.
filename	The file name of the destination SBMLR model definition file.

Value

No value returned.

Warning

SBML events and function definitions are NOT implemented.

Note

Similar to saveSBML, the file is written incrementally.

Author(s)

Tom Radivoyevitch

References

Radivoyevitch, T. A two-way interface between limited Systems Biology Markup Language and R. BMC Bioinformatics 5, 190 (2004).

See Also

saveSBML

Examples

```
library(SBMLR)
library(odesolve)
curto=readSBMLR(file.path(system.file(package="SBMLR"), "models/curto.r"))
saveSBMLR(curto,"curtoR.r")
curtoR=readSBMLR("curtoR.r")
curto==curtoR
summary(curtoR)
unlink("curtoR.r")
```

`simulate` *Simulate a model of class SBML*

Description

This function simulates a model given the report times and optional modulators. It uses `lsoda` of the odesolve package.

Usage

```
simulate(model, times, modulator=NULL,X0=NULL, ...)
```

Arguments

`model`	The model object to be simulated. Initial conditions are passed through this object.
`times`	The sequence of time points to be sampled and provided as rows of the output matrix.
`modulator`	Null if there are no modulators (default), a vector of numbers if there are steady state Vmax modulators, and a list of interpolating functions if there are time course Vmax modulators.
`X0`	Override model initial conditions in simulations, particularly piece-wise perturbation simulations.
`...`	For compatibility with `simulate` of the stats package.

Details

This is a wrapper for lsoda.

Value

The data frame output that comes out of `lsoda`.

Note

Rules are implemented through time varying boundary conditions updated at each time point as a side effect within the (now internal) function `fderiv`.

Author(s)

Tom Radivoyevitch

References

For the folate cycle example given below: Morrison PF, Allegra CJ: Folate cycle kinetics in human breast cancer cells. JBiolChem 1989, 264(18):10552-10566.

Examples

```
##---- The following example performs a perturbation in PRPP from 5 to 50 uM in Curto et
library(SBMLR)
library(odesolve)
curto=readSBML(file.path(system.file(package="SBMLR"), "models/curto.xml"))
out1=simulate(curto,seq(-20,0,1))
curto$species$PRPP$ic=50
out2=simulate(curto,0:70)
outs=data.frame(rbind(out1,out2))
attach(outs)
par(mfrow=c(2,1))
plot(time,IMP,type="l")
plot(time,HX,type="l")
par(mfrow=c(1,1))
detach(outs)

# which should be the same plots as
curto=readSBMLR(file.path(system.file(package="SBMLR"), "models/curto.r"))
out1=simulate(curto,seq(-20,0,1))
curto$species$PRPP$ic=50
out2=simulate(curto,0:70)
outs=data.frame(rbind(out1,out2))
attach(outs)
par(mfrow=c(2,1))
plot(time,IMP,type="l")
plot(time,HX,type="l")
par(mfrow=c(1,1))
detach(outs)

##---- The following example uses fderiv to generate Morrison's folate system response to

morr=readSBMLR(file.path(system.file(package="SBMLR"), "models/morrison.r"))
out1=simulate(morr,seq(-20,0,1))
morr$species$EMTX$ic=1
out2=simulate(morr,0:30)
outs=data.frame(rbind(out1,out2))
attach(outs)
par(mfrow=c(3,4))
plot(time,FH2b,type="l",xlab="Hours")
plot(time,FH2f,type="l",xlab="Hours")
plot(time,DHFRf,type="l",xlab="Hours")
plot(time,DHFRtot,type="l",xlab="Hours")
plot(time,CHOFH4,type="l",xlab="Hours")
plot(time,FH4,type="l",xlab="Hours")
plot(time,CH2FH4,type="l",xlab="Hours")
plot(time,CH3FH4,type="l",xlab="Hours")
plot(time,AICARsyn,type="l",xlab="Hours")
plot(time,MTR,type="l",xlab="Hours")
plot(time,TYMS,type="l",xlab="Hours")
#plot(time,EMTX,type="l",xlab="Hours")
plot(time,DHFReductase,type="l",xlab="Hours")
```

```
par(mfrow=c(1,1))
detach(outs)
morr$species$EMTX$ic=0
```

`summary.SBML` *Get summary information from an SBML model*

Description

This function extracts information from a model of class `SBML` and returns it as a list. The list includes species and reaction information tabularized as data frames.

Usage

```
## S3 method for class 'SBML'
summary(object,...)
```

Arguments

`object`	A model object of class `SBML` from which information is to be extracted.
`...`	For compatibility with `summary` of the base package.

Details

no details

Value

A list containing the following elements

`BC`	A logical vector indicating which species are not state variables, i.e. which species are boundary conditions or auxillary variables.
`y0`	The initial state (boundary conditions excluded!).
`nStates`	The length of the state vector, i.e. the number of system states.
`S0`	The full set of species initial values.
`nReactions`	The number of reactions.
`nSpecies`	The number of species, including states, boundary conditions and possibly auxillary variables such as the total concentration of dihydofolate reductase in the morrison.r model.
`incid`	The incidence/stoichiometry matrix. This usually contains ones and minus ones corresponding to fluxes either synthesizing or degrading (respectively) a state variable chemical species. This matrix multiplied by the flux vector on its right yields the corresponding concentration state variable time derivatives.
`species`	Species information (i.e. names, ICs, BCs, and compartments) as a data frame.
`reactions`	Reaction information tabularized as a dataframe, including string laws and initial fluxes.

Note

The list output can be attached to immediately define many model variables of interest.

Author(s)

Tom Radivoyevitch

Examples

```
library(SBMLR)
curto=readSBMLR(file.path(system.file(package="SBMLR"), "models/curto.r"))
summary(curto)
```

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