Copasi API 1.0

Generated by Doxygen 1.7.3

Mon Oct 3 2011 16:27:37

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# **Chapter 1**

# **Data Structure Index**

## 1.1 Data Structures

Here are the data structures with brief descriptions:

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# Chapter 2

# File Index

## 2.1 File List

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/home/deepak/copasi-simple-api/TC structs.h	?	?

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## **Chapter 3**

## **Data Structure Documentation**

## 3.1 copasi\_compartment Struct Reference

this struct is used to contain a pointer to an instance of a COPASI class #include <copasi\_api.h>

#### **Data Fields**

- void \* CopasiCompartmentPtr
- void \* CopasiModelPtr
- void \* qHash

## 3.1.1 Detailed Description

this struct is used to contain a pointer to an instance of a COPASI class Definition at line 42 of file copasi\_api.h.

The documentation for this struct was generated from the following file:

• /home/deepak/copasi-simple-api/copasi\_api.h

## 3.2 copasi\_model Struct Reference

this struct is used to contain a pointer to an instance of a COPASI class #include <copasi\_api.h>

## **Data Fields**

• home deepak copasi simple api copasi\_api h void \* CopasiModelPtr

- void \* CopasiDataModelPtr
- void \* qHash
- char \* errorMessage

## 3.2.1 Detailed Description

this struct is used to contain a pointer to an instance of a COPASI class Definition at line 25 of file copasi\_api.h.

The documentation for this struct was generated from the following file:

• /home/deepak/copasi\_simple-api/copasi\_api.h

## 3.3 copasi\_reaction Struct Reference

this struct is used to contain a pointer to an instance of a COPASI class

```
#include <copasi_api.h>
```

#### **Data Fields**

- void \* CopasiReactionPtr
- void \* CopasiModelPtr
- void \* qHash

## 3.3.1 Detailed Description

this struct is used to contain a pointer to an instance of a COPASI class Definition at line 34 of file copasi\_api.h.

The documentation for this struct was generated from the following file:

• /home/deepak/copasi-simple-api/copasi\_api.h

## 3.4 tc\_items Struct Reference

An array of int objects with length information. Use tc\_getItem(M,i) to get the i-th item.

```
#include <TC_structs.h>
```

## **Data Fields**

- int length
- long \* items

#### 3.4.1 Detailed Description

An array of int objects with length information. Use  $tc\_getItem(M,i)$  to get the i-th item

Definition at line 49 of file TC\_structs.h.

The documentation for this struct was generated from the following file:

• /home/deepak/copasi-simple-api/TC\_structs.h

## 3.5 tc\_matrix Struct Reference

A 2D table of doubles with row and column names. Use tc\_getMatrixValue(M,i,j) to get the i,j-th value in tc\_matrix M.

```
#include <TC_structs.h>
```

#### **Data Fields**

- int rows
- int cols
- double \* values
- tc\_strings rownames
- tc\_strings colnames

#### 3.5.1 Detailed Description

A 2D table of doubles with row and column names. Use  $tc\_getMatrixValue(M,i,j)$  to get the i,j-th value in  $tc\_matrix\ M$ .

Definition at line 57 of file TC\_structs.h.

The documentation for this struct was generated from the following file:

• /home/deepak/copasi-simple-api/TC\_structs.h

## 3.6 tc\_strings Struct Reference

An array of strings with length information. Use tc\_getString(M,i) to get the i-th string.

```
#include <TC_structs.h>
```

## **Data Fields**

- int length
- char \*\* strings

## 3.6.1 Detailed Description

An array of strings with length information. Use tc\_getString(M,i) to get the i-th string. Definition at line 41 of file TC\_structs.h.

The documentation for this struct was generated from the following file:

• /home/deepak/copasi-simple-api/TC\_structs.h

## 3.7 tc\_table Struct Reference

A 2D table of strings with row and column names. Use  $tc\_getTableValue(M,i,j)$  to get the i,j-th value in  $tc\_matrix\ M$ .

```
#include <TC_structs.h>
```

#### **Data Fields**

- int rows
- int cols
- char \*\* **strings**
- tc\_strings rownames
- tc\_strings colnames

## 3.7.1 Detailed Description

A 2D table of strings with row and column names. Use  $tc\_getTableValue(M,i,j)$  to get the i,j-th value in  $tc\_matrix\ M$ .

Definition at line 67 of file TC structs.h.

The documentation for this struct was generated from the following file:

• /home/deepak/copasi-simple-api/TC\_structs.h

## **Chapter 4**

## **File Documentation**

## 4.1 /home/deepak/copasi-simple-api/copasi\_api.h File Reference

```
Simple C API for the Copasi C++ library. #include "TC_structs.h"
```

## **Data Structures**

- struct copasi\_model

  this struct is used to contain a pointer to an instance of a COPASI class
- struct copasi\_reaction

  this struct is used to contain a pointer to an instance of a COPASI class
- struct copasi\_compartment

  this struct is used to contain a pointer to an instance of a COPASI class

## **Functions**

### Memory management

- TCAPIEXPORT void copasi\_end ()
   destroy copasi -- MUST BE CALLED at the end of program
- TCAPIEXPORT void cRemoveModel (copasi\_model)
   remove a model

## Read and write models

• TCAPIEXPORT copasi\_model cReadAntimonyFile (const char \*filename)

create a model from an Antimony or SBML file

- TCAPIEXPORT copasi\_model cReadSBMLFile (const char \*filename) create a model from an SBML file
- TCAPIEXPORT copasi\_model cReadSBMLString (const char \*sbml) create a model from an SBML string
- TCAPIEXPORT void cWriteSBMLFile (copasi\_model model, const char \*filename)

save a model as an SBML file

#### Create model

- TCAPIEXPORT copasi\_model cCreateModel (const char \*name) create a model
- TCAPIEXPORT void cCompileModel (copasi\_model model, int substitute\_nested assignments)

This function is only needed for calling COPASI methods not found in this library. This function compiles the COPASI model; it is called internally by the simulate and other anlysis functions.

- TCAPIEXPORT copasi\_compartment cCreateCompartment (copasi\_model model, const char \*name, double volume)
  - create compartment
- TCAPIEXPORT void cSetVolume (copasi\_model, const char \*compartment, double volume)

set a volume of compartment

• TCAPIEXPORT int cSetValue (copasi\_model, const char \*name, double value)

set the concentration of a species, volume of a compartment, or value of a parameter The function will figure out which using the name (fast lookup using hashtables). If the name does not exist in the model, a new global parameter will be created.

• TCAPIEXPORT void cCreateSpecies (copasi\_compartment compartment, const char \*name, double initialValue)

add a species to the model

 TCAPIEXPORT void cSetBoundarySpecies (copasi\_model model, const char \*species, int isBoundary)

set a species as boundary or floating (will remove any assignment rules)

- TCAPIEXPORT void cSetConcentration (copasi\_model, const char \*species, double value)
  - set a species as boundary or floating (will remove any assignment rules)

• TCAPIEXPORT int cSetAssignmentRule (copasi\_model model, const char \*species, const char \*formula)

set the assignment rule for a species (automatically assumes boundary species)

 TCAPIEXPORT int cSetGlobalParameter (copasi\_model model, const char \*name, double value)

set the value of an existing global parameter or create a new global parameter

• TCAPIEXPORT int cCreateVariable (copasi\_model model, const char \*name, const char \*formula)

create a new variable that is not a constant by a formula

• TCAPIEXPORT int cCreateEvent (copasi\_model model, const char \*name, const char \*trigger, const char \*variable, const char \*formula)

add a trigger and a response, where the response is defined by a target variable and an assignment formula

 TCAPIEXPORT copasi\_reaction cCreateReaction (copasi\_model model, const char \*name)

add a species or set an existing species as fixed

 TCAPIEXPORT void cAddReactant (copasi\_reaction reaction, const char \*species, double stoichiometry)

add a reactant to a reaction

• TCAPIEXPORT void cAddProduct (copasi\_reaction reaction, const char \*species, double stoichiometry)

add a product to a reaction

 TCAPIEXPORT int cSetReactionRate (copasi\_reaction reaction, const char \*formula)

set reaction rate equation

#### Time course simulation

• TCAPIEXPORT tc\_matrix cSimulateDeterministic (copasi\_model model, double startTime, double endTime, int numSteps)

simulate using LSODA numerical integrator

• TCAPIEXPORT tc\_matrix cSimulateStochastic (copasi\_model model, double startTime, double endTime, int numSteps)

simulate using exact stochastic algorithm

• TCAPIEXPORT tc\_matrix cSimulateHybrid (copasi\_model model, double startTime, double endTime, int numSteps)

simulate using Hybrid algorithm/deterministic algorithm

• TCAPIEXPORT tc\_matrix cSimulateTauLeap (copasi\_model model, double startTime, double endTime, int numSteps)

simulate using Tau Leap stochastic algorithm

## Steady state analysis

- TCAPIEXPORT tc\_matrix cGetSteadyState (copasi\_model model) bring the system to steady state
- TCAPIEXPORT tc\_matrix cGetSteadyState2 (copasi\_model model, int iter)

bring the system to steady state using normal simulation

- TCAPIEXPORT tc\_matrix cGetJacobian (copasi\_model model) get the Jacobian at the current state
- TCAPIEXPORT tc\_matrix cGetEigenvalues (copasi\_model model) get the eigenvalues of the Jacobian at the current state

#### Metabolic control analysis (MCA)

- TCAPIEXPORT tc\_matrix cGetScaledFluxControlCoeffs (copasi\_model model)
  - add a compartment to the model
- TCAPIEXPORT tc\_matrix cGetUnscaledElasticities (copasi\_model model) unscaled elasticities
- TCAPIEXPORT tc\_matrix cGetUnscaledConcentrationControlCoeffs (copasi\_model model)

unscaled elasticities

TCAPIEXPORT tc\_matrix cGetUnscaledFluxControlCoeffs (copasi\_model model)

unscaled flux control coefficients

- TCAPIEXPORT tc\_matrix cGetScaledElasticities (copasi\_model model) scaled elasticities
- TCAPIEXPORT tc\_matrix cGetScaledConcentrationConcentrationCoeffs (copasi\_model model)

 $scaled\ concentration\ control\ coefficients$ 

#### Stoichiometry matrix and matrix analysis

- TCAPIEXPORT tc\_matrix cGetFullStoichiometryMatrix (copasi\_model model)
  - full stoichiometry matrix
- TCAPIEXPORT tc\_matrix cGetReducedStoichiometryMatrix (copasi\_model model)

reduced stoichiometry matrix

TCAPIEXPORT tc\_matrix cGetElementaryFluxModes (copasi\_model model)

elementary flux modes

- TCAPIEXPORT tc\_matrix cGetGammaMatrix (copasi\_model model)
   get Gamma matrix (i.e. conservation laws)
- TCAPIEXPORT tc\_matrix cGetKMatrix (copasi\_model model) get K matrix (right nullspace)
- TCAPIEXPORT tc\_matrix cGetK0Matrix (copasi\_model model) get K0 matrix
- TCAPIEXPORT tc\_matrix cGetLinkMatrix (copasi\_model model) get L matrix (left nullspace)
- TCAPIEXPORT tc\_matrix cGetL0Matrix (copasi\_model model) get L0 matrix

## **Optimization (incomplete)**

TCAPIEXPORT tc\_matrix cOptimize (copasi\_model model, const char \*objective, tc\_matrix input)

fit the model parameters to time-series data

- TCAPIEXPORT void **cSetOptimizerIterations** (int)
- TCAPIEXPORT void **cSetOptimizerSize** (int)
- TCAPIEXPORT void **cSetOptimizerMutationRate** (double)
- TCAPIEXPORT void **cSetOptimizerCrossoverRate** (double)

### 4.1.1 Detailed Description

Simple C API for the Copasi C++ library. This is a C API for the COPASI C++ library. Rate equations in COPASI require the "complete name", e.g. instead of X, the rate must specify <model.compartment.X>. In this C API, those complete names are stored in a hash table. The API replaces the simple strings, i.e. "C", with the complete names by using the hash-table. This is mainly for speed; otherwise, every cSetReactionRate would be searching through the entire model for each of its variables. The hash-table idea is used for functions such as cSetValue, which can set the value of a parameter or that of a molecular species. Again, it uses the hash table to identify what a variable is.

The C API hides the C++ classes by casting some of the main classes into void pointers inside C structs.

std::map is used for performing the hashing (it is not a real hash-table, but close enough). boost::regex is used for string substitutions.

Definition in file copasi\_api.h.

#### 4.1.2 Function Documentation

## 4.1.2.1 TCAPIEXPORT void cAddProduct ( copasi\_reaction reaction, const char \* species, double stoichiometry )

add a product to a reaction

#### **Parameters**

copasi reaction	
char	* product
double	stoichiometry

## 4.1.2.2 TCAPIEXPORT void cAddReactant ( copasi\_reaction reaction, const char \* species, double stoichiometry )

add a reactant to a reaction

#### **Parameters**

copasi	reaction
reaction	
char	* reactant
double	stoichiometry

## 4.1.2.3 TCAPIEXPORT void cCompileModel ( copasi\_model model, int substitute\_nested\_assignments )

This function is only needed for calling COPASI methods not found in this library. This function compiles the COPASI model; it is called internally by the simulate and other anlysis functions.

#### **Parameters**

copasi	model
model	
int	substitute nested assignments

## 4.1.2.4 TCAPIEXPORT copasi\_compartment cCreateCompartment ( copasi\_model model, const char \* name, double volume )

create compartment

char*	compartment name

double	volume	1
--------	--------	---

#### Returns

copasi\_compartment a new compartment

## 4.1.2.5 TCAPIEXPORT int cCreateEvent ( copasi\_model model, const char \* name, const char \* trigger, const char \* variable, const char \* formula )

add a trigger and a response, where the response is defined by a target variable and an assignment formula

#### Parameters

copasi	model
model	
char	* event name
char	* trigger
char	* response: name of variable or species
char*	response: assignment formula

#### Returns

int 0=failed 1=success

## 4.1.2.6 TCAPIEXPORT copasi\_model cCreateModel ( const char \* name )

create a model

## **Parameters**

7	
char*	model name

#### Returns

copasi\_model a new copasi model

## 4.1.2.7 TCAPIEXPORT copasi\_reaction cCreateReaction ( copasi\_model model, const char \* name )

add a species or set an existing species as fixed

copasi	model
model	
char*	species name

#### Returns

copasi\_reaction a new reaction

## 4.1.2.8 TCAPIEXPORT void cCreateSpecies ( copasi\_compartment compartment, const char \* name, double initialValue )

add a species to the model

#### **Parameters**

copasi	model
compartment	
char*	species name
double	initial value (concentration or count, depending on the model)

## 4.1.2.9 TCAPIEXPORT int cCreateVariable ( copasi\_model model, const char \* name, const char \* formula )

create a new variable that is not a constant by a formula

#### **Parameters**

copasi	model
model	
char*	name of new variable
char*	formula

#### Returns

int 0=failed 1=success

## 4.1.2.10 TCAPIEXPORT tc\_matrix cGetEigenvalues ( copasi\_model model )

get the eigenvalues of the Jacobian at the current state

#### **Parameters**

copasi	model
model	

#### Returns

tc\_matrix matrix with 1 row and n columns, each containing an eigenvalue

#### 4.1.2.11 TCAPIEXPORT tc\_matrix cGetElementaryFluxModes ( copasi\_model model )

elementary flux modes

#### **Parameters**

copasi	model
model	

## Returns

tc\_matrix matrix with reactions as rows (with rownames) and flux modes as columns (no column names)

## 4.1.2.12 TCAPIEXPORT tc\_matrix cGetFullStoichiometryMatrix ( copasi\_model model )

full stoichiometry matrix

#### **Parameters**

copasi	model
model	

#### Returns

tc\_matrix

#### 4.1.2.13 TCAPIEXPORT tc\_matrix cGetGammaMatrix ( copasi\_model model )

get Gamma matrix (i.e. conservation laws)

## **Parameters**

```
copasi_- model
model
```

### Returns

tc\_matrix

### 4.1.2.14 TCAPIEXPORT tc\_matrix cGetJacobian ( copasi\_model model )

get the Jacobian at the current state

copasi	model
model	

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#### Returns

tc\_matrix matrix with n rows and n columns, where n = number of species

## 4.1.2.15 TCAPIEXPORT tc\_matrix cGetK0Matrix ( copasi\_model model )

get K0 matrix

#### **Parameters**

```
copasi_- model model
```

#### Returns

tc\_matrix

## 4.1.2.16 TCAPIEXPORT tc\_matrix cGetKMatrix ( copasi\_model model )

get K matrix (right nullspace)

#### **Parameters**

copasi	model
model	

#### Returns

tc\_matrix

## 4.1.2.17 TCAPIEXPORT tc\_matrix cGetL0Matrix ( copasi\_model model )

get L0 matrix

#### **Parameters**

```
copasi_- model model
```

#### Returns

tc\_matrix

## 4.1.2.18 TCAPIEXPORT tc\_matrix cGetLinkMatrix ( copasi\_model model )

get L matrix (left nullspace)

#### **Parameters**

```
copasi_- model
model
```

#### Returns

tc\_matrix

## 4.1.2.19 TCAPIEXPORT tc\_matrix cGetReducedStoichiometryMatrix ( copasi\_model model )

reduced stoichiometry matrix

#### **Parameters**

```
copasi_- model
model
```

#### Returns

tc\_matrix

## 4.1.2.20 TCAPIEXPORT tc\_matrix cGetScaledConcentrationConcentrationCoeffs ( copasi\_model model )

scaled concentration control coefficients

#### **Parameters**

```
copasi_- model
model
```

#### Returns

tc\_matrix

## 4.1.2.21 TCAPIEXPORT tc\_matrix cGetScaledElasticities ( copasi\_model model )

scaled elasticities

## **Parameters**

copasi -	model
model	
model	

#### Returns

tc\_matrix

#### 4.1.2.22 TCAPIEXPORT tc\_matrix cGetScaledFluxControlCoeffs ( copasi\_model model )

add a compartment to the model scaled flux control coefficients

#### **Parameters**

copasi	model/*! scaled flux control coefficients
model	
copasi	model
model	

#### Returns

tc\_matrix

#### **Parameters**

copasi	model
model	

#### Returns

tc\_matrix

## 4.1.2.23 TCAPIEXPORT tc\_matrix cGetSteadyState ( copasi\_model model )

bring the system to steady state

#### **Parameters**

copasi	model
model	

#### Returns

tc\_matrix matrix with 1 row and n columns, where n = number of species

#### 4.1.2.24 TCAPIEXPORT tc\_matrix cGetSteadyState2 ( copasi\_model model, int iter )

bring the system to steady state using normal simulation

copasi	model
model	
int	max iterations (each iteration doubles the time duration)

#### Returns

 $tc_{matrix}$  matrix with 1 row and n columns, where n = number of species

## 4.1.2.25 TCAPIEXPORT tc\_matrix cGetUnscaledConcentrationControlCoeffs ( copasi\_model model )

unscaled elasticities

unscaled concentration control coefficients

#### **Parameters**

copasi	model
model	

#### Returns

tc\_matrix

## 4.1.2.26 TCAPIEXPORT tc\_matrix cGetUnscaledElasticities ( copasi\_model model )

unscaled elasticities

## **Parameters**

```
copasi_- model model
```

#### Returns

tc\_matrix

#### 4.1.2.27 TCAPIEXPORT tc\_matrix cGetUnscaledFluxControlCoeffs ( copasi\_model model )

unscaled flux control coefficients

#### Parameters

conasi -	model
copusi_	model .
model	
mouet	

#### Returns

tc\_matrix

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## 4.1.2.28 TCAPIEXPORT tc\_matrix cOptimize ( copasi\_model model, const char \* objective, tc\_matrix input )

fit the model parameters to time-series data

#### **Parameters**

copasi	model
model	
char	* filename (tab separated)
tc_matrix	parameters to optimize. rownames should contain parameter names, col-
	umn 1 contains parameter min-values, and column 2 contains parameter
	max values
char	* pick method. Use of of the following: "GeneticAlgorithm", "Leven-
	bergMarquardt", "SimulatedAnnealing", "NelderMead", "SRES", "Parti-
	cleSwarm", "SteepestDescent", "RandomSearch"

use genetic algorithms to generate a distribution of parameter values that satisfy an objective function or fit a data file

## **Parameters**

	copasi	model
	model	
Ī	char	* objective function or filename
	tc_matrix	parameter initial values and min and max values (3 columns)

## 4.1.2.29 TCAPIEXPORT copasi\_model cReadAntimonyFile ( const char \* filename )

create a model from an Antimony or SBML file

#### **Parameters**

char*	file name

#### Returns

copasi\_model a new copasi model

## 4.1.2.30 TCAPIEXPORT $copasi\_model$ cReadSBMLFile ( const char \* filename )

create a model from an SBML file

\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	har*   fi	le name

#### Returns

copasi\_model a new copasi model

## 4.1.2.31 TCAPIEXPORT copasi\_model cReadSBMLString ( const char \* sbml )

create a model from an SBML string

#### **Parameters**

char*	SBML string
-------	-------------

#### Returns

copasi\_model a new copasi model

## 4.1.2.32 TCAPIEXPORT int cSetAssignmentRule ( copasi\_model model, const char \* species, const char \* formula )

set the assignment rule for a species (automatically assumes boundary species)

#### **Parameters**

copasi	model
model	
char	* species name
char*	formula, use 0 to remove assignment rule

#### Returns

int 0=failed 1=success

## 4.1.2.33 TCAPIEXPORT void cSetBoundarySpecies ( copasi\_model model, const char \* species, int isBoundary )

set a species as boundary or floating (will remove any assignment rules)

copasi	model
model	
char	* name
int	boundary = $1$ , floating = $0$ (default)

## 4.1.2.34 TCAPIEXPORT void cSetConcentration ( copasi\_model , const char \* species, double value )

set a species as boundary or floating (will remove any assignment rules)

#### **Parameters**

copasi	model
model	
char	* species name
double	concentration or count

## 4.1.2.35 TCAPIEXPORT int cSetGlobalParameter ( copasi\_model model, const char \* name, double value )

set the value of an existing global parameter or create a new global parameter

#### **Parameters**

copasi	model
model	
char*	parameter name
double	value

### Returns

int 0=new value created 1=found existing value

## 4.1.2.36 TCAPIEXPORT int cSetReactionRate ( copasi\_reaction reaction, const char \* formula )

set reaction rate equation

## **Parameters**

copasi	reaction
reaction	
char*	custom formula

#### Returns

int success=1 failure=0

## 4.1.2.37 TCAPIEXPORT int cSetValue ( copasi\_model , const char \* name, double value )

set the concentration of a species, volume of a compartment, or value of a parameter The function will figure out which using the name (fast lookup using hashtables). If the name does not exist in the model, a new global parameter will be created.

#### **Parameters**

copasi	model
model	
char	* name
double	value

#### Returns

0 if new variable was created. 1 if existing variable was found

## 4.1.2.38 TCAPIEXPORT void cSetVolume ( $copasi\_model$ , const char \* compartment, double volume)

set a volume of compartment

#### **Parameters**

copasi	model
model	
char	* compartment name
double	volume

## 4.1.2.39 TCAPIEXPORT tc\_matrix cSimulateDeterministic ( copasi\_model model, double startTime, double endTime, int numSteps )

simulate using LSODA numerical integrator

#### **Parameters**

copasi	model
model	
double	start time
double	end time
int	number of steps in the output

#### Returns

tc\_matrix matrix of concentration or particles

## 4.1.2.40 TCAPIEXPORT tc\_matrix cSimulateHybrid ( copasi\_model model, double startTime, double endTime, int numSteps )

simulate using Hybrid algorithm/deterministic algorithm

#### Parameters

1 urumevers	
copasi	model
model	

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double	start time
double	end time
int	number of steps in the output

## Returns

tc\_matrix matrix of concentration or particles

## 4.1.2.41 TCAPIEXPORT tc\_matrix cSimulateStochastic ( copasi\_model model, double startTime, double endTime, int numSteps )

simulate using exact stochastic algorithm

#### **Parameters**

copasi	model
model	
double	start time
double	end time
int	number of steps in the output

#### Returns

tc\_matrix matrix of concentration or particles

## 4.1.2.42 TCAPIEXPORT tc\_matrix cSimulateTauLeap ( copasi\_model model, double startTime, double endTime, int numSteps )

simulate using Tau Leap stochastic algorithm

#### **Parameters**

copasi	model
model	
double	start time
double	end time
int	number of steps in the output

## Returns

tc\_matrix matrix of concentration or particles

## 4.1.2.43 TCAPIEXPORT void cWriteSBMLFile ( copasi\_model model, const char \* filename )

save a model as an SBML file

copasi model	copasi model
char*	file name

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