

Copasi Simple API

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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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copasi_model (This struct is used to contain a pointer to an instance of a COPASI class)	6
copasi_reaction (This struct is used to contain a pointer to an instance of a COPASI class)	6

Chapter 2

File Index

2.1 File List

Here is a list of all files with brief descriptions:

copasi/[copasi_api.h](#) (Simple C API for the Copasi C++ library) 9

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

3.1.2 Field Documentation

3.1.2.1 void* CopasiCompartmentPtr

3.1.2.2 void* CopasiModelPtr

3.1.2.3 void* qHash

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

- [copasi/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 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

3.2.2 Field Documentation

3.2.2.1 void* CopasiDataModelPtr

3.2.2.2 home deepak copasi simple api copasi copasi_api h void* CopasiModelPtr

3.2.2.3 char* errorMessage

3.2.2.4 void* qHash

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

- [copasi/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

3.3.2 Field Documentation

3.3.2.1 void* CopasiModelPtr

3.3.2.2 void* CopasiReactionPtr

3.3.2.3 void* qHash

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

- [copasi/copasi_api.h](#)

Chapter 4

File Documentation

4.1 copasi/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 analysis 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 param-
eter The function will figure out which using the name (fast lookup using hashta-
bles). 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 [cGetKOMatrix](#) (copasi_model model)
get KO matrix
- TCAPIEXPORT tc_matrix [cGetLinkMatrix](#) (copasi_model model)
get L matrix (left nullspace)
- TCAPIEXPORT tc_matrix [cGetLOMatrix](#) (copasi_model model)
get LO 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.

QtCore is used for providing the hash-table feature and regular expression (QHash and QRegExp). This should be replaced with the boost library at some point.

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

<i>copasi_reaction</i>	reaction
<i>char</i>	* product
<i>double</i>	stoichiometry

4.1.2.2 TCAPIEXPORT void cAddReactant (copasi_reaction *reaction*, const char * *species*, double *stoichiometry*)

add a reactant to a reaction

Parameters

<i>copasi_reaction</i>	reaction
<i>char</i>	* reactant
<i>double</i>	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 analysis functions.

Parameters

<i>copasi_model</i>	model
<i>int</i>	substitute nested assignments

4.1.2.4 TCAPIEXPORT copasi_compartment cCreateCompartment (copasi_model *model*, const char * *name*, double *volume*)

create compartment

Parameters

<i>char*</i>	compartment name
--------------	------------------

<i>double</i>	volume
---------------	--------

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
<i>char</i>	* event name
<i>char</i>	* trigger
<i>char</i>	* response: name of variable or species
<i>char*</i>	response: assignment formula

Returns

int 0=failed 1=success

4.1.2.6 TCAPIEXPORT [copasi_model](#) cCreateModel (const char * *name*)

create a model

Parameters

<i>char*</i>	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

Parameters

copasi_model	model
<i>char*</i>	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_compartment	model
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

<i>copasi_- model</i>	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

<i>copasi_- model</i>	model
---------------------------	-------

Returns

tc_matrix

4.1.2.13 TCAPIEXPORT tc_matrix cGetGammaMatrix (copasi_model model)

get Gamma matrix (i.e. conservation laws)

Parameters

<i>copasi_- model</i>	model
---------------------------	-------

Returns

tc_matrix

4.1.2.14 TCAPIEXPORT tc_matrix cGetJacobian (copasi_model model)

get the Jacobian at the current state

Parameters

<i>copasi_- model</i>	model
---------------------------	-------

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

<i>copasi_model</i>	model
---------------------	-------

Returns

tc_matrix

4.1.2.16 TCAPIEXPORT tc_matrix cGetKMatrix (copasi_model model)

get K matrix (right nullspace)

Parameters

<i>copasi_model</i>	model
---------------------	-------

Returns

tc_matrix

4.1.2.17 TCAPIEXPORT tc_matrix cGetL0Matrix (copasi_model model)

get L0 matrix

Parameters

<i>copasi_model</i>	model
---------------------	-------

Returns

tc_matrix

4.1.2.18 TCAPIEXPORT tc_matrix cGetLinkMatrix (copasi_model model)

get L matrix (left nullspace)

Parameters

<i>copasi_- model</i>	model
---------------------------	-------

Returns

tc_matrix

4.1.2.19 TCAPIEXPORT tc_matrix cGetReducedStoichiometryMatrix (copasi_model model)

reduced stoichiometry matrix

Parameters

<i>copasi_- model</i>	model
---------------------------	-------

Returns

tc_matrix

4.1.2.20 TCAPIEXPORT tc_matrix cGetScaledConcentrationConcentrationCoeffs (copasi_model model)

scaled concentration control coefficients

Parameters

<i>copasi_- model</i>	model
---------------------------	-------

Returns

tc_matrix

4.1.2.21 TCAPIEXPORT tc_matrix cGetScaledElasticities (copasi_model model)

scaled elasticities

Parameters

<i>copasi_- model</i>	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

<i>copasi_model</i>	model/*! scaled flux control coefficients
<i>copasi_model</i>	model

Returns

tc_matrix

Parameters

<i>copasi_model</i>	model
---------------------	-------

Returns

tc_matrix

4.1.2.23 TCAPIEXPORT tc_matrix cGetSteadyState (copasi_model model)

bring the system to steady state

Parameters

<i>copasi_model</i>	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

Parameters

<i>copasi_model</i>	model
<i>int</i>	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

<i>copasi_model</i>	model
---------------------	-------

Returns

tc_matrix

4.1.2.26 TCAPIEXPORT tc_matrix cGetUnscaledElasticities (copasi_model model)

unscaled elasticities

Parameters

<i>copasi_model</i>	model
---------------------	-------

Returns

tc_matrix

4.1.2.27 TCAPIEXPORT tc_matrix cGetUnscaledFluxControlCoeffs (copasi_model model)

unscaled flux control coefficients

Parameters

<i>copasi_model</i>	model
---------------------	-------

Returns

tc_matrix

4.1.2.28 TCAPIEXPORT void copasi_end ()

destroy copasi -- MUST BE CALLED at the end of program

4.1.2.29 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
<i>char</i>	* filename (tab separated)
<i>tc_matrix</i>	parameters to optimize. rownames should contain parameter names, column 1 contains parameter min-values, and column 2 contains parameter max values
<i>char</i>	* pick method. Use of of the following: "GeneticAlgorithm", "LevenbergMarquardt", "SimulatedAnnealing", "NelderMead", "SRES", "ParticleSwarm", "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
<i>char</i>	* objective function or filename
<i>tc_matrix</i>	parameter initial values and min and max values (3 columns)

4.1.2.30 TCAPIEXPORT copasi_model cReadAntimonyFile (const char * filename)

create a model from an Antimony or SBML file

Parameters

<i>char*</i>	file name
--------------	-----------

Returns

[copasi_model](#) a new copasi model

4.1.2.31 TCAPIEXPORT copasi_model cReadSBMLFile (const char * filename)

create a model from an SBML file

Parameters

<i>char*</i>	file name
--------------	-----------

Returns

[copasi_model](#) a new copasi model

4.1.2.32 TCAPIEXPORT copasi_model cReadSBMLString (const char * *sbml*)

create a model from an SBML string

Parameters

<i>char*</i>	SBML string
--------------	-------------

Returns

[copasi_model](#) a new copasi model

4.1.2.33 TCAPIEXPORT void cRemoveModel (copasi_model)

remove a model

4.1.2.34 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
<i>char</i>	* species name
<i>char*</i>	formula, use 0 to remove assignment rule

Returns

int 0=failed 1=success

4.1.2.35 TCAPIEXPORT void cSetBoundarySpecies (copasi_model *model*, const char * *species*, int *isBoundary*)

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

Parameters

copasi_model	model
<i>char</i>	* name
<i>int</i>	boundary = 1, floating = 0 (default)

4.1.2.36 TCAPIEXPORT void cSetConcentration (copasi_model , const char * *species*, double *value*)

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

Parameters

<i>copasi_-model</i>	model
<i>char</i>	* species name
<i>double</i>	concentration or count

4.1.2.37 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

<i>copasi_-model</i>	model
<i>char*</i>	parameter name
<i>double</i>	value

Returns

int 0=new value created 1=found existing value

4.1.2.38 TCAPIEXPORT void cSetOptimizerCrossoverRate (double)

4.1.2.39 TCAPIEXPORT void cSetOptimizerIterations (int)

4.1.2.40 TCAPIEXPORT void cSetOptimizerMutationRate (double)

4.1.2.41 TCAPIEXPORT void cSetOptimizerSize (int)

4.1.2.42 TCAPIEXPORT int cSetReactionRate (copasi_reaction *reaction*, const char * *formula*)

set reaction rate equation

Parameters

<i>copasi_-reaction</i>	reaction
<i>char*</i>	custom formula

Returns

int success=1 failure=0

4.1.2.43 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

<i>copasi_model</i>	model
<i>char</i>	* name
<i>double</i>	value

Returns

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

4.1.2.44 TCAPIEXPORT void cSetVolume (copasi_model , const char * compartment, double volume)

set a volume of compartment

Parameters

<i>copasi_model</i>	model
<i>char</i>	* compartment name
<i>double</i>	volume

4.1.2.45 TCAPIEXPORT tc_matrix cSimulateDeterministic (copasi_model model, double startTime, double endTime, int numSteps)

simulate using LSODA numerical integrator

Parameters

<i>copasi_model</i>	model
<i>double</i>	start time
<i>double</i>	end time
<i>int</i>	number of steps in the output

Returns

tc_matrix matrix of concentration or particles

4.1.2.46 TCAPIEXPORT tc_matrix cSimulateHybrid (copasi_model *model*, double *startTime*, double *endTime*, int *numSteps*)

simulate using Hybrid algorithm/deterministic algorithm

Parameters

<i>copasi_model</i>	model
<i>double</i>	start time
<i>double</i>	end time
<i>int</i>	number of steps in the output

Returns

tc_matrix matrix of concentration or particles

4.1.2.47 TCAPIEXPORT tc_matrix cSimulateStochastic (copasi_model *model*, double *startTime*, double *endTime*, int *numSteps*)

simulate using exact stochastic algorithm

Parameters

<i>copasi_model</i>	model
<i>double</i>	start time
<i>double</i>	end time
<i>int</i>	number of steps in the output

Returns

tc_matrix matrix of concentration or particles

4.1.2.48 TCAPIEXPORT tc_matrix cSimulateTauLeap (copasi_model *model*, double *startTime*, double *endTime*, int *numSteps*)

simulate using Tau Leap stochastic algorithm

Parameters

<i>copasi_model</i>	model
<i>double</i>	start time

<i>double</i>	end time
<i>int</i>	number of steps in the output

Returns

tc_matrix matrix of concentration or particles

4.1.2.49 TCAPIEXPORT void cWriteSBMLFile (copasi_model *model*, const char * *filename*)

save a model as an SBML file

Parameters

<i>copasi_model</i>	copasi model
<i>char*</i>	file name

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