RoadRunner Documentation

Release 1.5.1

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Contents

CHAPTER 1

libRoadRunner Overview

This guide is intended as an introduction and reference of the RoadRunner SBML Simulation Engine. This guide will show the most important features and provides a complete API reference.

To get you started here is a very simple script that will load an example SBML model and run a time course simulation and plot the results:

```
import roadrunner

# load an SBML model
rr = roadrunner.RoadRunner("mymodel.xml")

# simulate from 0 to 10 time units with 100 output rows
result = rr.simulate(0,10,100)

rr.plot()
```

Looking for a model to start with? We included a couple with libRoadRunner, see *Loading Models*.

Note: The result is a standard numpy array which may be used with any numpy or scipy functions or may be plotted using matplotlib directly. See *Plotting Data* for help in plotting.

Now read the tutorials to learn more about the capabilities of RoadRunner.

Contents:

1.1 Introduction

1.1.1 Installing RoadRunner

Installing Manually

Windows

The installations instructions are updated regularly on the main website pages. Please refer to: http://libroadrunner.org/install#windows

Mac OS

The installations instructions are updated regularly on the main website pages. Please refer to: http://libroadrunner.org/install#mac

1.1.2 Basic Tutorial

Import RoadRunner

To startup RoadRunner use the commands at the Python prompt:

```
import roadrunner
rr = roadrunner.RoadRunner()
```

The variable `rr` is your reference to roadrunner. Anything you want to do with roadrunner must be specified using the variable `rr`.

To get the current version of libRoadRunner type the following:

```
roadrunner.__version__
```

Loading Models

RoadRunner reads models using the SBML format. If you have a SBML model stored on your hard drive, it is possible to load that model either by giving he document contents or path to the Roadrunner constructor, or later by using the method, *`load()`*. Let's assume you have a model called mymodel.xml in `C:\MyModels`. To load this model in **Windows** we would use the command:

```
rr = roadrunner.RoadRunner("C:/MyModels/mymodel.xml")
```

Note, Windows typically used the back slash, '' to indicate a directory separator, however in most languages including python, this is the escape character, therefore one can also enter Windows paths using the forward slash '/' which does not cause issues. If one want to use the backslash, these must be typed twice, i.e. `'C:\\MyModels\\mymodel.xml'`.

On the **Mac or Linux** we might use:

```
rr = roadrunner.RoadRunner("/home/MyModels/mymodel.xml")
```

RoadRunner can also load models directly from a URL via:

```
rr = roadrunner.RoadRunner("http://www.ebi.ac.uk/biomodels-main/download?
↪mid=BIOMD0000000010")
```

If the model was loaded successfully, the RoadRunner object is now ready to use, otherwise an exception will be raised that contains extended information detailing exactly what failed. If any warnings are found in the SBML document, these will be displayed in the console error log.

It is also possible to load a model from a string containing a SBML model, for example:

rr = roadrunner.RoadRunner (sbmlStr)

This is useful when one wishes to create a new roadrunner instance from an existing model, eg:

sbmlStr = rr.getCurrentSBML() rrnew = roadrunner.RoadRunner (sbmlStr)

Additionally, there are a couple models **included with libRoadRunner**. The models `feedback.xml` and `Test_1.xml` are available in the `roadrunner.testing` module. To access these use:

```
import roadrunner.testing as test
r = test.getRoadRunner('feedback.xml')
```

There are a few additional models in the `models/` directory of the distribution, where you installed libRoadRunner.

Running Simulations

Once a model is successfully loaded we can run a time course simulation. To run a simulation we use the *simulate()* method:

```
result = rr.simulate()
```

The output will be in a Python numpy array. The first column will contain time points and the remaining columns will include all the floating species amounts/concentrations. In the simulate method we didn't specify how long to run the simulation or how many points to generate. By default the starting time is set to zero, ending time to 10 and the number of points to 51. There are two ways to set these values. The easiest way is to change the positional arguments in *simulate()* in the following manner:

```
result = rr.simulate (0, 10, 100)
```

This will set the starting time to zero, the ending time to 10 and generate 100 points. This means that the result will be out in time intervals of 1/99.

The simulate method also accepts the steps keyword argument instead of points:

```
result = rr.simulate(0, 10, steps=99)
```

For more details of the simulate method see *simulate()*. The following table summarizes the various options.

Option	Description
start	Starting time for simulation
end	Ending time for simulation. Setting 'end' will automatically change 'duration'
points	Number of rows to include in the output matrix
selections	(Optional) A list of variables to include in the output, e.g. `['time','A']` for a model with species `A`. More below.
steps	(Optional keyword argument) Number of steps at which the output is sampled where the samples are evenly spaced. Steps = points-1. Steps and points may not both be specified.

One important point to note about *simulate()*: When *simulate()* is run, the concentration of the floating species will naturally change. If *simulate()* is called a second time, the simulation will start the simulation from the previous simulated values. This can be used to easily follow on simulations. However there will be times when we wish to run the same simulation again but perhaps with slightly different parameters values. For this we must reset the model to its initial conditions. To do that we run the command *reset()*:

```
rr.reset()
```

RoadRunner also has two other reset methods: *resetAll()* and *resetToOrigin()*. These are typically only used in advanced scenarios. This is because RoadRunner maintains its own copy of the "initial" value of every quantity, which can be set via `rr_instance.setValue('init(quantity)',123)`. When *resetAll()* is called, it resets the quantity to RoadRunner's internal copy, not the SBML-defined value. *resetToOrigin()* completely reverts everything in the model back to the SBML-specified values, whereas *resetAll()* preserves any changes you have made to initial values.

Changing Parameters

Often during a modeling experiment we will need to change parameter values, that is the values of the various kinetic constants in the model. If a model has a kinetic constants k1, then we can change or inspect the value using the following syntax:

```
print rr.k1
rr.k1 = 1.2
```

Selecting Simulation Output

RoadRunner supports a range of options for selecting what data a simulation should return. For more detailed information on selections, see the *Selecting Values* section.

The simulate method, by default returns an structured array, which are arrays that also contain column names. These can be plotted directly using the built in *plot()* function.

The output selections default to time and the set of floating species. It is possible to change the simulation result values by changing the selection list. For example assume that a model has three species, S1, S2, and S3 but we only want *simulate()* to return time in the first column and S2 in the second column. To specify this we would type:

```
rr.timeCourseSelections = ['time', 'S2']
result = rr.simulate (0, 10, 100)
```

In another example let say we wanted to plot a phase plot where S1 is plotted against S2. To do this we type the following:

```
rr.timeCourseSelections = ['S1', 'S2']
result = rr.simulate(0, 10, 100)
```

Some additional examples include:

```
# Select time and two rates of change (dS1/dt and dS2/dt)
rr.timeCourseSelections = ["time", "S1'", "S2'"]

# By default species names yield amounts, concentrations can be obtained
# using square brackets, e.g.
rr.timeCourseSelections = ['time', '[S1]', '[S2]']
```

See also:

More details on *Selecting Values*

Plotting Data

RoadRunner has a built in *plot()* method which can perform basic plotting. Simply call:

```
result = rr.simulate(0, 10, 100)
rr.plot()
```

If one wants more control over the data plots, one may use matplotlib directly. Assuming the simulate returns an array called result, and that the first column represents the x axis and the remaining columns the y axis, we type:

```
import pylab
pylab.plot (result[:,0],result[:,1:])
pylab.show()
```

This will bring up a new window showing the plot. To clear the plot for next time, type the command:

```
pylab.clf()
```

One may also override the built-in *plot()* method with a more more capable plotting routine.

Below is a simplified version of the *plot()* method. You may copy and write a customized version and even attach it to the RoadRunner object. The first argument is a RoadRunner object instance, and the second is a flag which tells the method to show the plot or not:

```
def plot(r, show=True):

    import pylab as p

    result = self.getSimulationData()

    if result is None:
        raise Exception("no simulation result")

    # assume result is a standard numpy array

    selections = r.timeCourseSelections

    if len(result.shape) != 2 or result.shape[1] != len(selections):
        raise Exception("simulation result columns not equal to number of selections,"
                        "likely a simulation has not been run")

    times = result[:,0]

    for i in range(1, len(selections)):
        series = result[:,i]
        name = selections[i]
        p.plot(times, series, label=str(name))

        p.legend()

    if show:
        p.show()
```

You can attach your plotting function to the RoadRunner object by simply setting the plot method:

```
def my_plot(r, show):
    pass

import roadrunner
roadrunner.RoadRunner.plot = my_plot
```

Now, whenever the *plot()* method is called, your plot function will be the one that is invoked.

Changing Initial Conditions

There are a number of methods to get and set the initial conditions of a loaded model. In order to specify a given initial conditions we use the notation, `init()`. The values stored in the initial conditions are applied to the model whenever it is reset. The list of all initial condition symbols can be obtained by the methods, *getFloatingSpeciesInitAmountIds()* and *getFloatingSpeciesInitConcentrationIds()* assuming `r` is a RoadRunner instance. As with all other selection symbols, the *keys()* returns all available selection symbols:

```
>>>  r.model.keys()
[ 'S1', 'S2', '[S1]', '[S2]', 'compartment', 'k1', '_CSUM0',
  'reaction1',  'init([S1])',  'init([S2])', 'init(S1)',
  'init(S2)',  "S1'"]
```

Symbols for selecting initial values specifically for amounts and concentrations can be obtained via:

```
>>> r.model.getFloatingSpeciesInitAmountIds()
['init(S1)', 'init(S2)']
```

```
>>> r.model.getFloatingSpeciesInitConcentrationIds()
['init([S1])', 'init([S2])']
```

Getting or setting initial values is easily accomplished using the array operator and the selection symbols:

```
>>> r.model["init(S1)"]
0.00015
```

```
>>> r.model["init([S1])"]
2.9999999999999997e-05
```

```
>>> r.model["init([S1])"] = 2
```

```
>>> r.model["init(S1)"]
10.0
```

The values for the initial conditions for all floating species can be obtained using the calls:

```
>>> r.model.getFloatingSpeciesInitConcentrations()
array([ 0.7,  5.6])
```

Initial conditions can be set using the two methods for all species in one call:

```
>>> r.model.setFloatingSpeciesInitAmounts ([3.4, 5.6])
```

```
>>> r.model.setFloatingSpeciesInitConcentrations ([6.7, 0.1])
```

Solvers

RoadRunner has multiple types of solvers including integrators and steady-state solvers. Integrators control numerical timecourse integration via the *simulate()* method. By default, RoadRunner uses CVODE, a real differential equation solver from the SUNDIALS suite. Internally, CVODE features an adaptive timestep. However, unless *variableStep* is specified in the call to *simulate()*, the output will contain evenly spaced intervals.

```
>>>  r.simulate(0, 10, 10)
# Output will contain evenly spaced intervals
>>>  r.simulate(variableStep=True)
# Intervals will vary according to CVODE step size
```

To use basic 4th-order Runge-Kutta integrator ('rk4'), call *setIntegrator()*:

```
>>>  r.setIntegrator('rk4')
```

Runge-Kutta always uses a fixed step size, and does not support events. RoadRunner supports Runge-Kutta-Fehlberg Method ('rkf45') as well as a stochastic integrator based on Gillespie algorithm ('gilliespie'). To get a list of all available integrators, run:

```
>>>  roadrunner.integrators
['cvode', 'gillespie', 'rk4', 'rk45']
```

Some integrators, such as CVODE, have parameters which can be set by the user. To see a list of these settings, use *getSettings()* on an integrator instance:

```
>>>  r.getIntegrator().getSettings()
('relative_tolerance',
'absolute_tolerance',
'stiff',
'maximum_bdf_order',
'maximum_adams_order',
'maximum_num_steps',
'maximum_time_step',
'minimum_time_step',
'initial_time_step',
'multiple_steps',
'variable_step_size')
```

To set a parameter, you can use both methods described below:

```
>>>  r.getIntegrator().relative_tolerance = 1e-10
>>>  r.getIntegrator().setValue('relative_tolerance', 1e-10)
```

Be sure to set the parameter to the correct type, which can be obtained from the parameter's hint or description:

```
>>>  r.getIntegrator().getHint('relative_tolerance')
'Specifies the scalar relative tolerance (double).'
>>>  r.getIntegrator().getDescription('relative_tolerance')
'(double) CVODE calculates a vector of error weights which is used in all error and␣
↪convergence tests. The weighted RMS norm for the relative tolerance should not␣
↪become smaller than this value.'
```

Parameters also have a display name:

```
>>>  r.getIntegrator().getDisplayName('relative_tolerance')
'Relative Tolerance'
```

If you prefer to change settings on integrators without switching the current integrator, you can use *getIntegratorByName()* as follows:

```
>>>  r.getIntegratorByName('gillespie').seed = 12345
```

Also, if you find yourself switching back and forth between integrators a lot, you can use *setIntegratorSetting()*.

```
>>>  r.setIntegratorSetting('gillespie', 'seed', 12345)
```

The other type of solver is a steady-state solver, which works in essentially the same way:

```
>>>  r.getSteadyStateSolver().getSettings()
('maximum_iterations',
'minimum_damping',
'relative_tolerance')
>>>  r.getSteadyStateSolver().getHint('maximum_iterations')
'The maximum number of iterations the solver is allowed to use (int)'
>>>  r.getSteadyStateSolver().getDescription('maximum_iterations')
'(int) Iteration caps off at the maximum, regardless of whether a solution has been␣
↪reached'
```

The steady state solver is invoked by a call to *steadyState()*. Currently, RoadRunner only has a single steady state solver (NLEQ).

1.1.3 What Is SBML?

The Systems Biology Markup Language (SBML) is a machine-readable language, based on XML, for representing models of biological processes. SBML can represent metabolic networks, cell-signaling pathways, regulatory networks, and many other kinds of systems. For more information, go to:

http://sbml.org/Main_Page

http://en.wikipedia.org/wiki/SBML

1.1.4 What is libRoadRunner

RoadRunner is a package for loading, simulating and analyzing SBML based systems biology models utilzing JIT compilation.

RoadRunner 1.4.3

Up to date documentation can be found on http://libroadrunner.org/.

Also documentation home page provides an introduction.

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http://libroadrunner.org/

Fundamental Objects

The libRoadRunner package uses two fundametal objects e.g. `rr` of class `RoadRunner` and e.g. `rr.model` of class `ExecutableModel`.

RoadRunner

- Typically the top level object
- Responsible for orchestrating all of the internal components, such as model loading, JIT compilation, integration and output.
- Initialized with `rr = roadrunner.RoadRunner()`

ExecutableModel

- Represents a compiled sbml model
- Properties to get and set any state variables.
- Initialized when SBML is loaded `r.load('mymodel.xml')`

The Python API is a very clean simple interface that uses all native Python objects. All the returned types are structured *Numpy* arrays.

Example of libRoadRunner in Use

Transcript from an Python session to demonstrate libRoadRunner use on this interactive Python console.

Import roardrunner and numpy:

```
import roadrunner
import roadrunner.testing
import numpy as n
import numpy.linalg as lin
```

Load an SBML model:

```
>>>  rr = roadrunner.RoadRunner()
>>>  rr.load(roadrunner.testing.get_data('Test_1.xml'))
True
```

Get the **model**, the model object has all the accessors sbml elements, names, values:

```
>>>  m = rr.getModel()
```

Use the built in RR function to get the **Jacobian**, notice this is returned as a native numpy matrix, and display it:

```
>>>  jac = rr.getFullJacobian()
>>>  jac
array([[-0.2  ,  0.067,  0.   ],
       [ 0.15 , -0.467,  0.09 ],
       [ 0.   ,  0.4  , -0.64 ]])
```

Get a vector of **floating species amounts**, and display it:

```
>>>  amt = m.getFloatingSpeciesAmounts()
>>>  amt
array([ 0.1 ,  0.25,  0.1 ])
```

Look at the **floating species ids**:

```
>>>  m.getFloatingSpeciesIds()
['S1', 'S2', 'S3']
```

Numpy has a huge amount of numeric capability, here we calculate the **eigensystem from the Jacobian**.:

```
>>>  lin.eig(jac)
(array([-0.15726345, -0.38237134, -0.76736521]),
 array([[ 0.77009381, -0.19510707,  0.03580588],
        [ 0.49121122,  0.53107368, -0.30320915],
        [ 0.40702219,  0.82455683,  0.95225109]]))
```

Suppose we wanted to calculate the matrix vector product of the **jacobian with the floating species amounts**, its a single statement, since we use native types.:

```
>>>  n.dot(jac, amt)
array([-0.00325, -0.09275,  0.036  ])
```

Finally, you can of course **simulate over time**. The first column in result is time, the rest are whatever is selected. The easies way to plot is to use `RoadRunner.plot()`:

```
>>>  results = rr.simulate()
>>>  rr.plot(results)
```

See also:

Plotting Data

Using libRoadRunner in IPython you can **get documentation** easily using a `?` after the object or method:

```
>>>  r.plot?

Type:        instancemethod
String form: <bound method RoadRunner.plot of <roadrunner.RoadRunner() { this =␣
↪0x101c70a00 }>>
File:        /Users/andy/Library/Python/2.7/lib/python/site-packages/roadrunner/
↪roadrunner.py
Definition:  r.plot(self, show=True)
Docstring:
RoadRunner.plot([show])

Plot the previously run simulation result using Matplotlib.

This takes the contents of the simulation result and builds a
legend from the selection list.


If the optional prameter 'show' [default is True] is given, the pylab
show() method is called.
```

Technical Footnotes

1.2 SBML Read/Write Functions

Use the following methods to read and write models in the form of SBML.

RoadRunner.load
RoadRunner.getCurrentSBML
RoadRunner.getSBML

1.3 Selecting Values

RoadRunner supports wide range of options for selecting SBML and derivative values. Selections can be used to either retrieve or store values. We define SBML values as any element specified in the original SBML document, whereas derivative values are a function of one or more SBML values. As these functions typically have no inverse, these are read only selections.

Selections are used a number of RoadRunner methods. They are used to determine what columns are selected in a simulation result and can also be used to directly select model values.

1.3.1 Selection syntax

The selection syntax is case sensitive (SBML elements are case sensitive), however it ignores all white space.

Selection Types:

Time: `time` The string `time` is interpreted as the current model time.

Identifier Any continuous sequence of printing characters is treated as an SBML identifier with the exception of `time`, i.e. `S1`, `P1`, `J0_Keq1`, `compartment`, etc. These have to be valid SBML identifiers. If no SBML identifier is found, an exception is raised. Note that if the identifier is a chemical species, it is interpreted as the species amount.

Concentration `[[]]` Following generally accepted chemical nomenclature, any continuous sequence of characters inside a pair of squared brackets, `[]` is interpreted as a concentration, i.e. `[S1]`, `[S2]`, etc. The identifier must be a valid SBML species, otherwise an exception is raised.

Rates of Change: `'` Represents the rate of change, $\frac{dy}{dt}$ of a species amount. Rates of change selections follow generally accepted mathematical convention of using the single quote, `'` to represent a time derivative. A rate of change selection is any identifier followed by a single quote, i.e. `S1'`, `S2'`, `P1'`, etc. A rates of change selection is also valid for SBML elements which are defined by rate rules. In Python, use mixture of single and double quote to specify the rates of change as string, e.g. `"S1'"`

Elasticity: `ee(ReactionId, ParameterId)` Represents elasticity slection in the form of `ee(ReactionId, ParameterId)` where `ReactionId` is a reaction name and `ParameterId` is a global parameter id. This selection intentionally has a function form, it selects the elasticity control coefficient, *`getEE()`*

Unscaled Elasticity: `uee(ReactionId, ParameterId)` Represents unscaled elasticity slection in the form of `uee(ReactionId, ParameterId)` where `ReactionId` is a reaction name and `ParameterId` is a global parameter id. This selection intentionally has a function form, it selects the elasticity control coefficient, *`getuEE()`*

Control Coefficient: `cc(Id, ParameterId)` Represents control coefficient selection in the form of `cc(Id, ParameterId)` where `Id` is a flux or species name and `ParameterId` is a global parameter id. The string `Id` and `ParameterId` must be valid arguments for *`getCC()`*. This selection intentionally has a function form, it selects the elasticity control coefficient, *`getCC()`*

Unscaled Control Coefficient: `ucc(Id, ParameterId)` Represents unscaled control coefficient selections in the form of `ucc(Id, ParameterId)` where *Id'* is a flux or species name and `ParameterId` is a global parameter id. The string `Id` and `ParameterId` must be valid arguments for *`getuCC()`*. This selection intentionally has a function form, it selects the unscaled elasticity control coefficient, *`getuCC()`*

Eigenvalue: `eigen(),eigenReal(),eigenImag()` Represents the eigenvalue of a floating species. `eigen(identifier)` is complex number whereas `eigenReal(identifier)` is the real part of eigenvalue and `eigenImag(identifier)` is the imaginary part of eigenvalue.

Initial Value: `init()` Represents the initial value of an identifier (species or global parameter) specified in the SBML document, i.e. `init(S1)`. Setting this value does not reset the *current* value of the quantity. When

`resetAll()` is called, the current values of all quantities will be reset to the designated initial values, including any changes made to the initial values via this syntax. This is in contrast to `resetToOrigin()`, which resets all current and initial values to the values specified in the SBML document.

Stoichiometry: `stoich(ParameterId, ReactionId)` Represents the stoichiometric coefficient for a given species and reaction.

Experimenting With Selections

One might try individual selection string using the *`getValue()`* method. This takes a selection string, determines if it is valid, and returns the value it selects. For example:

```
>>> rr.getValue("cc(S1, J4_KS4)")
-0.42955738179207886
```

Even though they are almost always specified by a string, RoadRunner selections are actually objects. One can create a selection object using *`createSelection()`*. In order to see extended information about the selection, try:

```
>>> sel = rr.createSelection("cc(S1, J4_KS4)")
>>> sel
SelectionRecord({'index' : -1, 'p1' : 'S1', 'p2' : 'J4_KS4', 'selectionType' :␣
↪CONTROL})
```

We can see that this is a CONTROL record.

It is also possible to modify the simulation selection list by deleting existing items and adding new ones created with *`createSelection()`*. If someone has does not want to display the concentration of species `S2` and instead wants to display the rate of change of species `S1`, try:

```
>>> rr.timeCourseSelections
["time", "[S1]", "[S2]", "[S3]", "[S4]"]

>>> sel = rr.createSelection("S1'")
>>> rr.timeCourseSelections[2] = sel
>>> rr.timeCourseSelections
["time", "[S1]", "S1'", "[S3]", "[S4]"]
```

Even though the selection list intentionally appears as a list of strings, it is actually a list of selection objects. So, elements that are inserted or appended to this list must be selection objects created by *`createSelection()`*.

Selecting Simulation Results

The columns of the RoadRunner simulation results are determined by the *`timeCourseSelections`* property. This is a list of what values will be displayed in the result, and can be set simply by:

```
>>>  rr.timeCourseSelections = ['time', '[S1]', 'S1', "S1'"]
```

This example selects the columns `time`, concentration of `S1`, amount of `S1`, and rate of change of `S1`. One may also have derivative values in the simulation selection, for example, if one wanted to plot the elasticity of a particular reaction `J1`:

```
>>>  rr.timeCourseSelections = ['time', '[S1]', "ee(J1, P1)"]
```

1.3.2 Methods and properties which accept selections

ExecutableModel.__getitem__
ExecutableModel.__setitem__

1.4 Steady State Analysis

The dynamics of a biochemical network is described by the system equation

$$\frac{d}{dt}\mathbf{s}(t) = \mathbf{N}\mathbf{v}(\mathbf{s}(t), \mathbf{p}, t),$$

where $\mathbf{s}$ is the vector of species concentrations, $\mathbf{p}$ is a vector of time independent parameters, and t is time. The steady state is the solution to the network equations when all the rates of change are zero. That is the concentrations of the floating species, $\mathbf{s}$ that satisfy:

$$\mathbf{N}\mathbf{v}(\mathbf{s}(t), \mathbf{p}, t) = 0$$

The steady state is easily calculated using the steady state method:

```
>>> rr.steadyState()
1.234567E-9
```

The call to `steadyState` returns a value that represents the sum of squares of the rates of change. Therefore the smaller this value the more likely the steady state solution has been found. Often a value less that 10E-6 indicates a steady state has been found. After a successful call all the species levels will be at their steady state values.

Steady state values can be obtained using *getSteadyStateValues()* and *steadyStateSelections()* can be used to decide what values to return. For example the following would retrieve a single value:

```
>>> rr.steadyStateSelections = ['S1']
>>> rr.getSteadyStateValues()
array([ 0.54314239])
```

One important element in running steady state analysis is the concept of moiety conservation. If the model in question contains moiety conserved cycles, traditional approach to obtain steady state solution fails as it is impossible to calculate the inverse of Jacobian. In such case, we use a walkaround and split the species in a cycle into groups. To do this in RoadRunner, type:

```
>>> rr.conservedMoietyAnalysis = True
```

Currently, RoadRunner only support `nleq1` solver for performing steady state analysis. This will be expanded in the future, and we included framework to select different solvers for steady state analysis. To set the solver and see all settings, type:

```
>>> rr.setSteadyStateSolver('nleq')
>>> solver = rr.getSteadyStateSolver()
>>> solver.settingsPyDictRepr()
"'maximum_iterations': 100, 'minimum_damping': 1e-16, 'relative_tolerance': 0.0001"
```

To see all available steady state solvers, type:

```
>>> rr.getRegisteredSteadyStateSolverNames()
('nleq',)
```

The following methods deal with steady state analysis:

RoadRunner.steadyStateSelections
RoadRunner.steadyState
RoadRunner.getSteadyStateValues
RoadRunner.conservedMoietyAnalysis

1.5 Stochastic Simulation

RoadRunner supports stochastic simulation through the use of Gillespie algorithm, which is a variation of Monte Carlo method.

To set the current instance of RoadRunner to use the Gillespie solver, try:

```
>>>  rr.setIntegrator('gillespie')
```

RoadRunner also supports a simplified method to run Gillespie solver through *gillespie()*.

One of the important component of stochastic simulation is setting the seed. Random number genetration in computers are known to be 'pseudo-random', meaning it can only 'approximate' randomness. Seed is an initial key value for generating a sequence of numbers. This means that when a seed is given, it is possible to regenerate identical sequence of numbers from random number generator. This might be desireable for reproducibility perposes but undesireable for multiple iterations of random number creation.

By using *getSettings()*, you can check settings accepted by Gillespie solver.

```
>>>  rr.getIntegrator().getSettings()
('seed',
 'variable_step_size',
 'initial_time_step',
 'minimum_time_step',
 'maximum_time_step',
 'nonnegative')
```

For information on what the settings represent, try *getDescription()*. Check *Solvers* for additional information.

The following methods deal with stochastic simulation:

RoadRunner.gillespie

1.6 Stoichiometric Analysis

1.6.1 Preliminaries

A network of m chemical species and n reactions can be described by the m by n stochiometry matrix $\mathbf{N}$. $\mathbf{N}_{i,j}$ is the net number of species i produced or consumed in reaction j. The dynamics of the network are described by

$$\frac{d}{dt}\mathbf{s}(t) = \mathbf{N}\mathbf{v}(\mathbf{s}(t), \mathbf{p}, t),$$

where $\mathbf{s}$ is the vector of species concentrations, $\mathbf{p}$ is a vector of time independent parameters, and t is time.

Each structural conservation, or interchangably, *conserved sum* (e.g. conserved moiety) in the network coresponds to a lineraly dependent row in the stoichiometry matrix $\mathbf{N}$.

If there are conserved sums, then the row rank, r of N is $< m$, and the stochiometry matrix N may first be re-ordered such that the first r are linearly independent, and the remaining $m - r$ rows are linear combinations of the first r rows. The *reduced stochiometry matrix* $\mathbf{N_R}$ is then formed from the first r rows of N. Finally, N may be expressed as a product of the $m \times r$ *link matrix* $\mathbf{L}$ and the $r \times n$ $\mathbf{N_R}$ matrix:

$$\mathbf{N} = \mathbf{L}\mathbf{N}_\mathbf{R}.$$

The link matrix $\mathbf{L}$ has the form

$$\mathbf{L} = \begin{bmatrix} \mathbf{I}_r \\ \mathbf{L}_0 \end{bmatrix},$$

where $\mathbf{I}_r$ is the $r \times r$ identity matrix and $\mathbf{L}_0$ is a $(m - r) \times r$ matrix.

1.6.2 Full vs. Extended Stoichiometry Matrix

The "full" stoichiometric matrix includes any conserved quantities (as opposed to the reduced stoichiometric matrix, which does not). The *extended* stoichiometric matrix is equal to the full stoichiometric matrix plus additional rows representing boundary species and sources / sinks. For example, consider the following reaction system:

```
reaction1:  => C
reaction2: C =>
reaction3: C =>
reaction4: MI => M
reaction5: M => MI
reaction6: XI => X
reaction7: X => XI
```

The extended stoichiometry matrix for this system is:

```
>>>  rr.getExtendedStoichiometryMatrix()
                     reaction1, reaction2, reaction3, reaction4, reaction5, reaction6,
↪ reaction7
 C                 [[         1,        -1,        -1,         0,         0,         0,
↪          0],
 M                  [         0,         0,         0,         1,        -1,         0,
↪          0],
 X                  [         0,         0,         0,         0,         0,         1,
↪         -1],
 MI                 [         0,         0,         0,        -1,         1,         0,
↪          0],
 XI                 [         0,         0,         0,         0,         0,        -1,
↪          1],
 reaction1_source   [        -1,         0,         0,         0,         0,         0,
↪          0],
 reaction2_sink     [         0,         1,         0,         0,         0,         0,
↪          0],
 reaction3_sink     [         0,         0,         1,         0,         0,         0,
↪          0]]
```

1.6.3 Methods

The following methods are related to the analysis of the stoichiometric matrix.

RoadRunner.getLinkMatrix
RoadRunner.getNrMatrix
RoadRunner.getKMatrix
RoadRunner.getConservationMatrix
RoadRunner.getL0Matrix
RoadRunner.getFullStoichiometryMatrix
RoadRunner.getExtendedStoichiometryMatrix
RoadRunner.getReducedStoichiometryMatrix
ExecutableModel.getNumConservedMoieties
ExecutableModel.getConservedMoietyIds
ExecutableModel.getConservedMoietyValues
ExecutableModel.setConservedMoietyValues

1.7 Metabolic Control Analysis

1.7.1 Preliminaries

Metabolic control analysis is the study of how sensitive the system is to pertubrations in parameters and how those perturbations progagate through the network. Two kinds of sensitivity are defined, system and local. The local sensitivities are described by the elasticities. These are defined as follows:

$$\varepsilon_S^v = \frac{\partial v}{\partial S}\frac{S}{v} = \frac{\partial \ln v}{\partial \ln S}$$

Given a reaction rate v_i, the elasticity describes how a given effector of the reaction step affects the reaction rate. Because the definition is in terms of partial deriviatives, any effector that is perturbed assumes that all other potential effectors are unchanged.

The system sensitivities are described by the control and response coefficients. These come in two forms, flux and concentration. The flux control coefficients measures how senstive a given flux is to a perturbation in the local rate of a reaction step. Often the local rate is perturbed by changing the enzyme concentration at the step. In this siutation the flux control coefficicent with respect to enzyme E_i is defined as follow:

$$C_{E_i}^J = \frac{dJ}{dE_i}\frac{E_1}{J} = \frac{d\ln J}{d\ln E_i}$$

Likewise the concentration control coefficient is defined by:

$$C_{E_i}^S = \frac{dS}{dE_i}\frac{E_1}{S} = \frac{d\ln S}{d\ln E_i}$$

where S is a given species. The response coefficients measure the sensitivity of a flux or species concentration to a perturbation in some external effector. These are defined by:

$$R_X^J = \frac{dJ}{dX}\frac{X}{J} = \frac{d\ln J}{d\ln X}$$

$$R_X^S = \frac{dJ}{dX}\frac{X}{S} = \frac{d\ln S}{d\ln X}$$

where X is the external effector.

1.7.2 Methods

The following methods allow users to obtain various metabolic control coefficients.

This first block of methods are for parameter independent coefficients.

RoadRunner.getUnscaledFluxControlCoefficientMatrix
RoadRunner.getUnscaledConcentrationControlCoefficientMatrix
RoadRunner.getUnscaledElasticityMatrix
RoadRunner.getUnscaledSpeciesElasticity
RoadRunner.getScaledElasticityMatrix
RoadRunner.getScaledFloatingSpeciesElasticity
RoadRunner.getScaledFluxControlCoefficientMatrix
RoadRunner.getScaledConcentrationControlCoefficientMatrix

Use these to obtain metabolic control coefficients.

RoadRunner.getuCC
RoadRunner.getCC
RoadRunner.getDiffStepSize
RoadRunner.setDiffStepSize
RoadRunner.getuEE
RoadRunner.getEE

1.8 Stability Analysis

The stability of a biochemical system is determined by the eigenvalues of the Jacobian matrix. Given m floating species and n reactions, the Jacobian matrix is defined as follows:

$$J = \begin{bmatrix} \frac{\partial F_1}{\partial S_1} & \cdots & \frac{\partial F_1}{\partial S_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_n}{\partial S_1} & \cdots & \frac{\partial F_n}{\partial S_m} \end{bmatrix}$$

where F_i is the ith differential equation and S_i the ith floating species. From RoadRunner it is easy to obtain the Jacobian matrix using *getFullJacobian()*, i.e.:

```
Jac = rr.getFullJacobian()
```

which returns the Jacobian matrix in the variable Jac.

It is possible for full Jacobian to be singular. In these situations one should call the related method, *getReducedJacobian()*.

1.9 Bifurcation Analysis

Bifurcation analysis is useful for understanding model with multiple steady states. RoadRunner supports bifurcation analysis through rrplugins package, which is an extension package to RoadRunner and provides an interface to AUTO2000.

Start using rrplugins package by importing the library and creating a Plugin instance.

```
>>> from rrplugins import *
>>> auto = Plugin("tel_auto2000")
```

The Plugin instance will have various properties you can set. For example, to load a model:

```
>>> sbmlModel = "path/to/SBML/model/"
>>> auto.setProperty("SBML", readAllText(sbmlModel))
```

To change number maximum number of steps:

```
>>> auto.setProperty("NMX", 5000)
```

To change the scan direction:

```
>>> auto.setProperty("ScanDirection", "Positive")
```

To change principal continuation parameter as well as its lower and upper bounds:

```
>>> auto.setProperty("PrincipalContinuationParameter", A)
>>> auto.setProperty("PCPLowerBound", 10)
>>> auto.setProperty("PCPUpperBound", 200)
```

Execute the plugin by running:

```
>>> auto.execute()
```

rrplugins package comes with several plotting functions as well, which is espeicially useful for plotting bifucation diagrams with ease. After executing the plugin, results will be stored in `BifurcationPoints`, `BifurcationLabels`, and `BifurcationData`. You can use these information to plot a bifurcation diagram.

```
>>> pts     = auto.BifurcationPoints
>>> lbls    = auto.BifurcationLabels
>>> biData  = auto.BifurcationData
>>> biData.plotBifurcationDiagram(pts, lbls)
```

To see the full list of properties, go to rrplugins AUTO2000 documentation

1.10 Accessing the SBML Model Variables

The following methods allow users to obtain information on the model

1.10.1 Compartments

ExecutableModel.getCompartmentVolumes
ExecutableModel.getNumCompartments
ExecutableModel.getCompartmentIds
ExecutableModel.setCompartmentVolumes

1.10.2 Boundary Species

ExecutableModel.getBoundarySpeciesConcentrations
ExecutableModel.setBoundarySpeciesConcentrations
ExecutableModel.getNumBoundarySpecies
ExecutableModel.getBoundarySpeciesIds

1.10.3 Floating Species

ExecutableModel.getFloatingSpeciesConcentrations
ExecutableModel.setFloatingSpeciesConcentrations
ExecutableModel.getNumFloatingSpecies
ExecutableModel.getFloatingSpeciesIds

1.10.4 Initial Conditions

ExecutableModel.getFloatingSpeciesInitAmountIds
ExecutableModel.getFloatingSpeciesInitConcentrationIds
ExecutableModel.getFloatingSpeciesInitAmounts
ExecutableModel.setFloatingSpeciesInitAmounts
ExecutableModel.getFloatingSpeciesInitConcentrations
ExecutableModel.setFloatingSpeciesInitConcentrations

1.10.5 Reactions

ExecutableModel.getNumReactions
ExecutableModel.getReactionRates
ExecutableModel.getReactionIds

1.10.6 Reaction Rates

ExecutableModel.getFloatingSpeciesAmountRates
ExecutableModel.getReactionRates
ExecutableModel.getNumReactions
ExecutableModel.getReactionIds

1.10.7 Global Parameters

ExecutableModel. setGlobalParameterValues
ExecutableModel. getGlobalParameterValues
ExecutableModel. getNumGlobalParameters
ExecutableModel. getNumGlobalParameters

1.11 Simulation and Integration

1.11.1 Preliminaries

At the highest level, RoadRunner generates and solves ODE (ordinary differential equation) problem of the form

$$y(t) = \int_0^t f(t, y)dt$$

where the function :math: f(t) is generated from the SBML document.

As this is numerically integrated, it is impossible to specify a time step and other integration parameters that are ideal for all functions. As a general rule for numeric stability, if you have a periodic function, you need a time step that is approximately 1/12 the period.

There are a number of tuning parameters that allows one to fine tune the numeric integration to their function at hand. We have chosen a set of precision values that we feel are a good balance between performance and numeric stability for most systems. However, one may frequently encounter stiffer systems which require tighter tolerances . Note that specifying very tight tolerances will drastically decrease performance.

Another parameter which is a significant role in numeric stability and performance is the initial time step. If no initial time step is provided (initial time step < 0, the default value), the internal integrator (defaults to CVODE) will estimate an initial time step based on total time span and and other numeric attributes calculated from the system. If the estimated initial time step is too large, then a significant amount of time will be spent by the integrator adjusting it down to a stable value. If the initial time step is too small, the integrator will waste needless steps re-evaluating the system function. As we use variable time step integrators, the time step will increase if the function is relatively smooth, however, by the time the time step has been increased, the simulation time may be over.

If one encounters exceptions from the integrator, the first thing that one should try is specifying an initial time step and tighter absolute and relative tolerances.

All of the parameters to tune the integration are specified on the integrator object:

```
>>>  r=roadrunner.RoadRunner("mymodel.xml")
```

Now specify absolute and relative tolerances

```
>>>  r.integrator.absolute_tolerance = 5e-10
>>>  r.integrator.relative_tolerance = 1e-3
```

and specify initial time step.

```
>>>  r.integrator.initial_time_step = 0.00001
>>>  r.simulate(0, 10)
```

This will specify the absolute and relative tolerances and initial time step, and will integrate the system from time 0 to 10. The internal integrator will take many time steps before it reaches time 10.

1.12 Utility Functions

The following methodsprovide basic information about the current roadRunner installation.

1.12.1 Information Group

getInfo() returns useful information about libRoadRunner's current state:

```
>>> print rr.getInfo()
Model Loaded: false
ConservationAnalysis: 0
libSBML version: LibSBML Version: 5.12.0
Temporary folder: not used
Compiler location: not used
Support Code Folder: not used
Working Directory: C:\dev\eclipse
```

getVersionStr() returns specific information Strings based on arguments passed to it. For example to get the libSBML version used, you can:

```
>>> import roadrunner

>>> print roadrunner.getVersionStr(roadrunner.VERSIONSTR_LIBSBML)
LibSBML Version: 5.9.0
```

or you can do any combination of the *VERSIONSTR_* options:

```
>>> print roadrunner.getVersionStr(
                            roadrunner.VERSIONSTR_BASIC |
                            roadrunner.VERSIONSTR_COMPILER |
                            roadrunner.VERSIONSTR_DATE |
                            roadrunner.VERSIONSTR_LIBSBML)
1.4.3; Compiler: Microsoft Visual Studio 2013; Date: Dec 18 2013, 22:59:30; LibSBML␣
↪Version: 5.12.0
```

There is also the standard python `__version__` which is actually set when the module is loaded from `getVersionStr`:

```
>>> print roadrunner.__version__
1.4.3; Compiler: Microsoft Visual Studio 2013; Date: Dec 18 2013, 22:59:30
```

RoadRunner.getInfo

1.13 RoadRunner API Reference

This is the API Reference page for the module: *roadrunner* The RoadRunner SBML Simulation Engine Python API, (c) 2009-2016 Endre Somogyi and Herbert Sauro

1.13.1 Configuration

Many of RoadRunner classes use a number of configuration parameters. Most of these can be set using the Config class. The values stored in the Config class only determine the *default* values of parameters. The Config class will look in the following locations for the config file, and will load the values from the first config file it finds. If it does not find a config file in one of the following locations, a default set of configuration parameters are used. The search locations of the config file are:

#1: the ROADRUNNER_CONFIG environment variable

#2: try the user's home directory for roadrunner.conf, i.e.:

```
/Users/andy/roadrunner.conf
```

#3: try the user's home directory for .roadrunner.conf, i.e.:

```
/Users/andy/.roadrunner.conf
```

#4: try the same directory as the roadrunner shared library, this will be the same directory as the python _roadrunner.pyd python extension module, i.e.:

```
/Users/andy/local/lib/roadrunner.conf
```

#5: try one directory up from the where the shared library or program is at, i.e.:

```
/Users/andy/local/roadrunner.conf
```

The conf file is just a plain text file of where each line may be key / value pair separated by a ":", i.e.

```
KEY_NAME : Value
```

Any line that does not match this format is ignored, and keys that are not found are also ignored. Therefore, any line that does not start with a word character is considered a comment.

All of the configuration management functions are static method of the Config class, and all of the configuration keys are static attributes of the Config class, these are documented in the Configuration Functions section.

As all of the Config class methods are static, one never instantiates the Config class.

Configuration Functions

static Config.**setValue**(*key*, *value*)

Set the value of a configuration key. The value must be either a string, integer, double or boolean. If one wanted to turn off moiety conservation (this will not have an effect on already loaded models):

```
from roadrunner import Config
Config.setValue(Config.LOADSBMLOPTIONS_CONSERVED_MOIETIES, False)
```

Or, other options may be set to Boolean or integer values. To enable an optimization features:

```
Config.setValue(Config.LOADSBMLOPTIONS_OPTIMIZE_INSTRUCTION_SIMPLIFIER, True)
```

static Config.**getConfigFilePath**()

If roadrunner was able to find a configuration file on the file system, its full path is returned here. If no file was found, this returns a empty string.

static Config.**readConfigFile**(*path*)
Read all of the values from a configuration file at the given path. This overrides any previously stored configuration. This allows users to have any number of configuration files and load them at any time. Say someone had to use Windows, and they had a file in their C: drive, this would be loaded via:

```
Config.readConfigFile("C:/my_config_file.txt")
```

Note, the forward slash works on both Unix and Windows, using the forward slash eliminates the need to use a double back slash, "\".

static Config.**writeConfigFile**(*path*)
Write all of the current configuration values to a file. This could be written to one of the default locations, or to any other location, and re-loaded at a later time.

Available Configuration Parameters

All of the configuration parameter keys are static attributes of the Config class and are listed here. The variable type of the parameter is listed after the key name.

Config.**LOADSBMLOPTIONS_CONSERVED_MOIETIES bool**
Perform conservation analysis. By default, this attribute is set as False.

This causes a re-ordering of the species, so results generated with this flag enabled can not be compared index wise to results generated otherwise.

Moiety conservation is only compatible with simple models which do NOT have any events or rules which define or alter any floating species, and which have simple constant stoichiometries.

Moiety conservation may cause unexpected results, be aware of what it is before enabling.

Not recommended for time series simulations.

To enable, type:

```
>>> roadrunner.Config.setValue(roadrunner.Config.LOADSBMLOPTIONS_CONSERVED_
↪MOIETIES, True)
```

Config.**LOADSBMLOPTIONS_RECOMPILE bool**
Should the model be recompiled? The LLVM ModelGenerator maintains a hash table of currently running models. If this flag is NOT set, then the generator will look to see if there is already a running instance of the given model and use the generated code from that one.

If only a single instance of a model is run, there is no need to cache the models, and this can safely be enabled, realizing some performance gains.

Config.**LOADSBMLOPTIONS_READ_ONLY bool**
If this is set, then a read-only model is generated. A read-only model can be simulated, but no code is generated to set model values, i.e. parameters, amounts, values, etc...

It takes a finite amount of time to generate the model value setting functions, and if they are not needed, one may see some performance gains, especially in very large models.

Config.**LOADSBMLOPTIONS_MUTABLE_INITIAL_CONDITIONS bool**
Generate accessors functions to allow changing of initial conditions.

Config.**LOADSBMLOPTIONS_OPTIMIZE_GVN bool**
GVN - This pass performs global value numbering and redundant load elimination contemporaneously.

Config.**LOADSBMLOPTIONS_OPTIMIZE_CFG_SIMPLIFICATION bool**
CFGSimplification - Merge basic blocks, eliminate unreachable blocks, simplify terminator instructions, etc...

Config.**LOADSBMLOPTIONS_OPTIMIZE_INSTRUCTION_COMBINING bool**
InstructionCombining - Combine instructions to form fewer, simple instructions. This pass does not modify the CFG, and has a tendency to make instructions dead, so a subsequent DCE pass is useful.

Config.**LOADSBMLOPTIONS_OPTIMIZE_DEAD_INST_ELIMINATION bool**
DeadInstElimination - This pass quickly removes trivially dead instructions without modifying the CFG of the function. It is a BasicBlockPass, so it runs efficiently when queued next to other BasicBlockPass's.

Config.**LOADSBMLOPTIONS_OPTIMIZE_DEAD_CODE_ELIMINATION bool**
DeadCodeElimination - This pass is more powerful than DeadInstElimination, because it is worklist driven that can potentially revisit instructions when their other instructions become dead, to eliminate chains of dead computations.

Config.**LOADSBMLOPTIONS_OPTIMIZE_INSTRUCTION_SIMPLIFIER bool**
InstructionSimplifier - Remove redundant instructions.

Config.**LOADSBMLOPTIONS_USE_MCJIT bool**
Currently disabled.

Use the LLVM MCJIT JIT engine.

Defaults to false.

The MCJIT is the new LLVM JIT engine, it is not as well tested as the original JIT engine. Does NOT work on LLVM 3.1

Config.**ROADRUNNER_DISABLE_PYTHON_DYNAMIC_PROPERTIES int**
RoadRunner by default dynamically generates accessors properties for all SBML symbol names on the model object when it is retrieved in Python. This feature is very nice for interactive use, but can slow things down. If this feature is not needed, it can be disabled here.

Config.**ROADRUNNER_DISABLE_WARNINGS int**
Disable SBML conserved moiety warnings.

Conserved Moiety Conversion may cause unexpected behavior, be aware of what it is before enabling.

RoadRunner will issue a warning in steadyState if conservedMoieties are NOT enabled because of a potential singular Jacobian. To disable this warning, set this value to 1

A notice will be issued whenever a document is loaded and conserved moieties are enabled. To disable this notice, set this value to 2.

To disable both the warning and notice, set this value to 3

Rationale for these numbers: This is actual a bit field, disabling the steady state warning value is actually 0b01 << 0 which is 1, and the loading warning is 0b01 << 1 which is 2 and 0b01 & 0b10 is 0b11 which is 3 in decimal.

Config.**LOADSBMLOPTIONS_PERMISSIVE int**
Accept some non-valid SBML (such as Booleans in numberic expressions).

For legacy code only. Do not use.

Config.**MAX_OUTPUT_ROWS int**
Set the maximum number of rows in the output matrix.

For models with very fine time stepping, the output of simulate can use up all available memory and crash the system. This option provides an upper bound on the maximum number of rows the output can contain. The simulation will be aborted and the output truncated if this value is exceeded.

Config.**ALLOW_EVENTS_IN_STEADY_STATE_CALCULATIONS bool**
Enable or disable steady state calculations when a model contains events

If true, steady state calculations will be carried out irrespective of whether events are present or not. If false, steady state calculations will not be carried out in the presence of events.

1.13.2 The Main RoadRunner Class

class roadrunner.**RoadRunner**

The main RoadRunner class. Its objects, i.e. `rr = RoadRunner()` perform the libRoaRunner functions, i.e. `rr.simulate()`.

RoadRunner.**__init__**(*uriOrSBML = ""*, *options = None*)

Creates a new RoadRunner object. If the first argument is specified, it should be a string containing either the contents of an SBML document, or a formatted URI specifying the path or location of a SBML document.

If options is given, it should be a LoadSBMLOptions object.

If no arguments are given, a document may be loaded at any future time using the load method.

Parameters

- **uriOrSBML** – a URI, local path or SBML document contents.
- **options** – (LoadSBMLOptions) an options object specifying how the SBML document should be loaded

RoadRunner.**load**(*uriOrDocument*)

Loads an SBML document, given a string for file path, URI, or contents.

This method also accepts HTTP URI for remote files, however this feature is currently limited to the Mac version, plan on enabling HTTP loading of SBML documents on Windows and Linux shortly.

Some examples of loading files on Mac or Linux:

```
>>> r.load("myfile.xml")                                    # load a file from the␣
↪current directory
>>> r.load("/Users/Fred/myfile.xml")                        # absolute path
>>> r.load("http://sbml.org/example_system.xml")            # remote file
```

Or on Windows:

```
>>> r.load("myfile.xml")                                      # load a file from the␣
↪current directory
>>> r.load("file://localhost/c:/Users/Fred/myfile.xml")     # using a URI
```

One may also load the contents of a document:

```
>>> myfile = open("myfile.xml, "r")
>>> contents = file.read()
>>> r.load(contents)
```

Loading in a raw SBML string is also possible:

```
>>> sbmlstr = rr.getCurrentSBML()          # Or any other properly formatted SBML␣
↪string block
>>> r.load(sbmlstr)
```

In future version, we will also support loading directly from a libSBML Document object.

Parameters **uriOrDocument** – A string which may be a local path, URI or contents of an SBML document.

RoadRunner.**saveState**(*document*, *option = 'b'*)

Saves the current state of the RoadRunner instance, e.g. integrator, steady state solver, simulation results, given a string for file path. If no option is given or the option is 'b', the state will be stored in a binary format which

can be quickly reloaded for later simulation. This binary format is platform specific. It the option is 'r', the state will be stored in a human-readable format which can be used for debugging, but cannot be reloaded later.

Some examples of saving binary files on Mac or Linux:

```
>>> r.saveState("current_state.txt")                          # save the state to a␣
↪file from the current directory
>>> r.saveState("/Users/Fred/current_state.txt")              # absolute path
```

Or on Windows:

```
>>> r.saveState("current_state.txt")                          # save the state to a␣
↪file from the current directory
>>> r.saveState("file://localhost/c:/Users/Fred/current_state.txt")    # using a␣
↪URI
```

One may also save in a human-readable format:

```
>>> r.saveState("current_state.txt", 'r')
```

Parameters

- **document** – The file path where the current state will be stored
- **option** – an option object specifying how the state should be saved 'b' - binary (default) 'r' - human-readable

RoadRunner.**loadState**(*document*)

Loads the saved state of a RoadRunner instance, e.g. integrator, steady state solver, simulation results, given a string for file path. All simulation calls after this function will start from the resumed state.

Some examples of reloading binary files on Mac or Linux:

```
>>> r.loadState("current_state.txt")                          # load the state from␣
↪a file from the current directory
>>> r.loadState("/Users/Fred/current_state.txt")              # absolute path
```

Or on Windows:

```
>>> r.loadState("current_state.txt")                          # load the state from␣
↪a file from the current directory
>>> r.loadState("file://localhost/c:/Users/Fred/current_state.txt")    # using a␣
↪URI
```

Parameters **document** – The file path where the state of simulation will be loaded from

RoadRunner.**getCompiler**()

Returns the JIT *Compiler* object currently being used. This object provides various information about the current processor and system.

RoadRunner.**getConfigurationXML**()

Recurse through all of the child configurable objects that this class ones and build an assemble all of their configuration parameters into a single xml document which is returned as a string.

The value of this result depends on what child objects are presently loaded.

RoadRunner.**getExtendedVersionInfo**()

Returns `getVersionStr()` as well as info about dependent libs versions.

RoadRunner.**getInfo**()
Returns info about the current state of the object.

Return type str

RoadRunner.**getInstanceCount**()
Returns number of currently running RoadRunner instances.

RoadRunner.**getInstanceID**()
Returns the instance id when there are multiple instances of RoadRunner.

RoadRunner.**getIntegrator**()
Returns the solver instance. See `roadrunner.Solver`. For more information on the possible settings, see *Solvers*.

RoadRunner.**getIntegratorByName**(*name*)
Returns the solver instance by given name. See `roadrunner.Solver`. For more information on the possible settings, see *Solvers*.

Parameters **name** (*str*) – Name of the integrator

RoadRunner.**getAvailableIntegrators**()
Returns a list of names of available integrators.

RoadRunner.**getExistingIntegratorNames**()
Returns a list of names of all integrators.

RoadRunner.**getParamPromotedSBML**(**args*)
Takes an SBML document (in textual form) and changes all of the local parameters to be global parameters.

Parameters **SBML** (*str*) – the contents of an SBML document

Return type str

RoadRunner.**getCurrentSBML**()
Returns the SBML with the current model parameters. This is different than *getSBML()* which returns the original SBML. This may optionally up or down-convert the document to a different version, if the level and version arguments are non-zero. If both arguments are zero, then the document is left alone and the original version is returned.

Return type str

RoadRunner.**getSBML**()
Returns the original SBML model that was loaded into roadrunner. If the model is edited by methods in editing section, it will return the most updated model with the initial model parameters.

Return type str

RoadRunner.**setIntegrator**(*name*)
Sets specific integrator. For more information on the possible settings, see *Solvers*.

Parameters **name** (*str*) – name of the integrator.

RoadRunner.**setIntegratorSetting**(*name*, *key*, *value*)
Sets settings for a specific integrator. See `roadrunner.Solver`. For more information on the possible settings, see *Solvers*.

Parameters

- **name** (*str*) – name of the integrator.
- **key** (*str*) – name of the setting.
- **value** (*const*) – value of the setting.

Selections

RoadRunner.**getIds**()
Return a list of selection ids that this object can select on.

Return type list

RoadRunner.**getValue**(*sel*)
Returns the value for a given selection. For more information on accepted selection types see *Selecting Values*.

Parameters **sel** (*str or SelectionRecord*) – a selection that is either a string or a SelectionRecord that was obtained from createSelection

RoadRunner.**getSelectedValues**()
returns the values of the current timecourse selections for the current state of the model

Return type numpy.ndarray

RoadRunner.**timeCourseSelections**
Get or set the list of current selections used for the time course simulation result columns. For more information on accepted selection types, see *Selecting Values*.

```
>>> rr.timeCourseSelections = ['time', 'S1', 'S2']
>>> rr.timeCourseSelections
['time', 'S1', 'S2']
```

RoadRunner.**createSelection**(*sel*)
Create a new selection based on a selection string

Return type *roadrunner.SelectionRecord*

RoadRunner.**resetSelectionLists**()
Resets time course and steady state selection lists to defaults

Model Access

RoadRunner.**isModelLoaded**()
Return True if model was loaded; False otherwise

RoadRunner.**model None**
Get the currently loaded model. The model object contains the entire state of the SBML model.

RoadRunner.**getModel**()
Function form of the RoadRunner.model property, identical to model.

RoadRunner.**clearModel**()
Clears the currently loaded model and all associated memory. Returns True if memory was freed, False if no model was loaded in the first place.

```
>>> r.isModelLoaded()
True
>>> r.clearModel()
>>> r.isModelLoaded()
False
```

RoadRunner.**oneStep**(*startTime*, *stepSize*)
Carry out a one step integration of the model. The method takes two arguments, the current time and the step size to use in the integration. Returs the new time which will be currentTime + StepSize:

```
newTime = rr.oneStep (10, 0.5)
```

RoadRunner.**internalOneStep**(*startTime*, *stepSize*, *reset*)
Carry out a single internal solver integration step. The method takes three arguments, the current time and the step size to use in the integration and reset. Reset defaults to true, set to false to stop integrator instance from restarting. Returns the end time.

RoadRunner.**reset**()
Resets time, all floating species, and rates to their initial values. Does NOT reset changed global parameters.

RoadRunner.**resetAll**()
Resets time, all floating species, and rates to their CURRENT initial values. Also resets all global parameters back to the values they had when the model was first loaded. "Current" initial values are set by using `r.setValue('init(S1)', 5)` which sets a species named S1 to have current initial value of 5. Note it is NOT the initial values of when the model was first loaded in.

RoadRunner.**resetParameter**()
Resets only global parameters to their CURRENT initial values.

RoadRunner.**resetToOrigin**()
Resets the model back to the state it was when FIRST loaded. The scope of this reset includes all initial values and parameters (everything).

RoadRunner.**setConfigurationXML**(**args*)
Given a xml document, which should have been returned from getConfigurationXML, this method recurses though all the child configurable elements and sets their configuration to the values specified in the document.

Parameters **xml** (*str*) – the contents of an xml document.

RoadRunner.**conservedMoietyAnalysis**
Enables / Disables conserved moiety analysis (boolean).

If this is enabled, the SBML document (either current, or one about to be loaded) is converted using the ConservedMoietyConverter. All of the linearly dependent species are replaced with assignment rules and a new set of conserved moiety parameters are introduced.

To enable, type:

```
>>> r.conservedMoietyAnalysis = True
```

Model Editing

Easy edit to the model without modifying and reloading sbml files.

RoadRunner.**addSpecies**(*sid*, *compartment*, *initValue*, *substanceUnits*, *forceRegenerate*)
Add a species to the current model. Note that the species to be added must have an ID that did not existed in the model. The given compartment must also exist in the model.

Default substanceUnits is "concentration", which will set initValue as initial concentration of the new species. Other substanceUnits will set initValue as initial amount of the new species.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addSpecies("s1", "compartment", 0.1, "concentration", false) # it will not␣
↪regenerate the model, nothing actually happened
>>> r.addSpecies("s2", "compartment", 0.1, "concentration", true)  # new model is␣
↪generated and saved
```

Parameters

- **sid** (*str*) – the ID of the species to be added
- **compartment** (*str*) – the compartment of the species to be added
- **initValue** (*double*) – the initial amount or concentration of the species to be added
- **substanceUnits** (*str*) – the substance unit of the species to be added
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**removeSpecies**(*sid*, *forceRegenerate*)

Remove a species from the current model. Note that the given species must exist in the current model.

All reactions related to this species(as reactants, products or modifiers or used in stoichiometry) will be removed. Kinetic law used this species in the math formula will be unset. All function definitions, constraints, initial assignments and rules related to this species (as variables or used in math formula) will be removed. All events used this speices in trigger formula will be removed. Priority and delay used this sepcies in the math formula will be unset. All event assignment related to this species(as variables or used in math formula) will be removed.

If any global parameters become uninitialized during this process, i.e, has no initial assignment or assignment rule, they will be removed recursively following the rules in removeParameter().

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.removeSpecies("s1", false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.removeSpecies("s2", true)  # new model is generated and saved
```

Parameters

- **sid** (*str*) – the ID of the species to be removed
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addReaction**(*rid*, *reactants*, *products*, *kineticLaw*, *forceRegenerate*)

Add a reaction to the current model by passing its info as parameters. Note that the reaction to be added must have an ID that did not existed in the model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addReaction("r1", ["s1"], ["s2"], "s1 * k1", false) # it will not␣
↪regenerate the model, nothing actually happened
>>> r.addReaction("r2", ["s2"], ["s1"], "s2 * k1", true)  # new model is␣
↪generated and saved
```

Parameters

- **rid** (*str*) – the ID of the reaction to be added
- **reactants** (*list*) – the list of reactants ID of reaction to be added
- **products** (*list*) – the list of products ID of reaction to be added
- **kineticLaw** (*str*) – the kinetic formular of reaction to be added
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addReaction**(*sbmlRep*, *forceRegenerate*)

Add a reaction to the current model by passing a sbml repesentation as parameter. Note that the reaction to be added must have an ID that did not existed in the model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

Parameters

- **sbmlRep** (*str*) – the SBML representation (i.e. a reaction tag) describing the reaction to be added
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**removeReaction**(*rid*, *forceRegenerate*)

Remove a reaction from the current model. Note that the given reaction must exist in the current model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.removeReaction("r1", false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.removeReaction("r2", true)  # new model is generated and saved
```

Parameters

- **rid** (*str*) – the ID of the reaction to be removed
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addParameter**(*pid*, *value*, *forceRegenerate*)

Add a parameter to the current model. Note that the parameter to be added must have an ID that did not existed in the model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addParameter("p1", 0.1, false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.addParameter("p2", 0.1, true)  # new model is generated and saved
```

Parameters

- **pid** (*str*) – the ID of the parameter to be added
- **value** (*double*) – the initial value of the parameter to be added
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**removeParameter**(*pid*, *forceRegenerate*)

Remove a parameter from the current model. Note that the given parameter must exist in the current model.

All reactions related to this parameter(used in stoichiometry) will be removed. Kinetic law used this parameter in the math formula will be unset. All function definitions, constraints, initial assignments and rules related to this parameter (as variables or used in math formula) will be removed. All events used this parameter in trigger formula will be removed. Priority and delay used this parameter in the math formula will be unset. All event assignment related to this parameter(as variables or used in math formula) will be removed.

If any global parameters become uninitialized during this process, i.e, has no initial assignment or assignment rule, they will be removed recursively following the above rules.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.removeParameter("p1", false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.removeParameter("p2", true)  # new model is generated and saved
```

Parameters

- **pid** (*str*) – the ID of the parameter to be removed
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addCompartment**(*cid*, *initVolume*, *forceRegenerate*)

Add a compartment to the current model. Note that the compartment to be added must have an ID that did not existed in the model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addCompartment("c1", 0.1, false) # it will not regenerate the model,␣
↪nothing actually happened
>>> r.addCompartment("c2", 0.1, true)  # new model is generated and saved
```

Parameters

- **cid** (*str*) – the ID of the compartment to be added
- **initVolume** (*double*) – the initial volume of the compartment to be added
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**removeCompartment**(*cid*, *forceRegenerate*)

Remove a compartment from the current model. Note that the given compartment must exist in the current model.

All reactions related to this compartment(used in stoichiometry) will be removed. Kinetic law used this compartment in the math formula will be unset. All function definitions, constraints, initial assignments and rules related to this compartment (as variables or used in math formula) will be removed. All events used this compartment in trigger formula will be removed. Priority and delay used this compartment in the math formula will be unset. All event assignment related to this compartment(as variables or used in math formula) will be removed.

If any global parameters become uninitialized during this process, i.e, has no initial assignment or assignment rule, they will be removed recursively following the rules in removeParameter().

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.removeCompartment("c1", false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.removeCompartment("c2", true)  # new model is generated and saved
```

Parameters

- **cid** (*str*) – the ID of the compartment to be removed
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**setKineticLaw**(*rid*, *kineticLaw*, *forceRegenerate*)

Set hte kinetic law for an existing reaction in the current model. Note that given reaction must exist in the model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.setKineticLaw("r1", "s1 * k1", false) # it will not regenerate the model,␣
↪nothing actually happened
>>> r.setKineticLaw("r2", "s2 * k1", true)  # new model is generated and saved
```

Parameters

- **rid** (*str*) – the ID of the reaction to be modified
- **kineticLaw** (*str*) – the kinetic formular of reaction to be set
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addAssignmentRule**(*vid*, *formula*, *forceRegenerate*)

Add an assignment rule for a variable to the current model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addAssignmentRule("s1", "s1 * k1", false) # it will not regenerate the␣
↪model, nothing actually happened
>>> r.addAssignmentRule("s2", "s2 * k1", true)  # new model is generated and saved
```

Parameters

- **vid** (*str*) – the ID of the variable that the new rule assigns formula to
- **formula** (*str*) – the math formula of assignment rule to be added
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addRateRule**(*vid*, *formula*, *forceRegenerate*)

Add a rate rule for a variable to the current model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addRateRule("s1", "k1", false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.addRateRule("s2", "k1", true)  # new model is generated and saved
```

Parameters

- **vid** (*str*) – the ID of the variable that the new rule assigns formula to
- **formula** (*str*) – the math formula of rate rule to be added
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**removeRules**(*vid*, *forceRegenerate*)

Remove all rules for a variable from the current model, including assignment and rate rules. Note that the given variable must have at least one rule in the current model.

If any global parameters become uninitialized during this process, i.e, has no initial assignment or assignment rule, they will be removed recursively following the rules in removeParameter().

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.removeRules("s1", false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.removeRules("s2", true)  # new model is generated and saved
```

Parameters

- **vid** (*str*) – the ID of the variables that rules assign formula to
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addEvent**(*eid*, *useValuesFromTriggerTime*, *trigger*, *forceRegenerate*)

Add an event to the current model. Note that the event to be added must have an ID that did not existed in the model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addEvent("e1", false, "s1 > 0", false) # it will not regenerate the model,␣
↪nothing actually happened
>>> r.addEvent("e2", false, "s2 == s1", true)  # new model is generated and saved
```

Parameters

- **eid** (*str*) – the ID of the event to be added
- **useValuesFromTriggerTime** (*bool*) – indicate the moment at which the event's assignments are to be evaluated
- **trigger** (*str*) – the math formula of event trigger
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addTrigger**(*eid*, *trigger*, *forceRegenerate*)

Add trigger to an existing event in the model. Note that the given event must exist in the current model. If the given event already has a trigger object, the given trigger will replace the old trigger of the event.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addTrigger("e1", "s1 > 0", false) # it will not regenerate the model,␣
↪nothing actually happened
>>> r.addTrigger("e2", "s2 == s1", true)  # new model is generated and saved
```

Parameters

- **eid** (*str*) – the ID of the event to add the trigger to
- **trigger** (*str*) – the math formula of event trigger
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addPriority**(*eid*, *priority*, *forceRegenerate*)

Add priority to an existing event in the model. Note that the given event must exist in the current model. If the given event already has a priority object, the given priority will replace the old priority of the event.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

Parameters

- **eid** (*str*) – the ID of the event to add the priority to
- **priority** (*str*) – the math formula of event priority
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addDelay**(*eid*, *delay*, *forceRegenerate*)

Add delay to an existing event in the model. Note that the given event must exist in the current model. If the given event already has a delay object, the given delay will replace the old delay of the event.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

Parameters

- **eid** (*str*) – the ID of the event to add the delay to
- **delay** (*str*) – the math formula of event delay
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**addEventAssignment**(*eid*, *vid*, *formula*, *forceRegenerate*)

Add an event assignment to an existing event in the model. Note that the given event must exist in the current model.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.addEventAssignment("e1", "s1", "k1", false) # it will not regenerate the␣
↪model, nothing actually happened
>>> r.addEventAssignment("e2", "s2", "s1", true)  # new model is generated and␣
↪saved
```

Parameters

- **eid** (*str*) – the ID of the event to add the event assignment to
- **vid** (*str*) – the ID of the variables that assignment assigns formula to
- **formula** (*str*) – the math formula of event assignment
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**removeEventAssignment**(*eid*, *vid*, *forceRegenerate*)

Add all event assignments for a variable from an existing event in the model. Note that the given event must exist in the current model and given variable must have an event assignment in the given event.

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.removeEventAssignment("e1", "s1", false) # it will not regenerate the model,
↪ nothing actually happened
>>> r.removeEventAssignment("e2", "s2", true)  # new model is generated and saved
```

Parameters

- **eid** (*str*) – the ID of the event
- **vid** (*str*) – the ID of the variables of the event assignments to be removed
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

RoadRunner.**removeEvent**(*eid*, *forceRegenerate*)

Add an event from the current model. Note that the given event must exist in the current model.

If any global parameters become uninitialized during this process, i.e, has no initial assignment or assignment rule, they will be removed recursively following the rules in removeParameter().

forceRegenerate is a boolean value that indicates whether the new model will be regenerated. Its default value is true, which means to regenerate model every time after this function is called. Note that regenerating model is time-consuming. To save time for editing model for multiple times, one could set this flag to false excepting for the last call, so that Roadrunner will only regenerate the model once after all editings are completed.

For example,

```
>>> r.removeEvent("e1", false) # it will not regenerate the model, nothing␣
↪actually happened
>>> r.removeEvent("e2", true)  # new model is generated and saved
```

Parameters

- **eid** (*str*) – the ID of the event to be removed
- **forceRegenerate** (*bool*) – indicate whether the new model is regenerated after this function call

Simulation

Fast and easy time series simulations is one of the main objectives of the RoadRunner project.

All simulation related tasks can be accomplished with the single `simulate` method.

`RoadRunner.`**`simulate`**(**args*, ***kwargs*)

Simulate and optionally plot current SBML model. This is the one stop shopping method for simulation and plotting.

simulate accepts a up to four positional arguments.

The first four (optional) arguments are treated as:

1: Start Time, if this is a number.

2: End Time, if this is a number.

3: Number of points, if this is a number.

4: List of Selections. A list of variables to include in the output, e.g. `['time','A']` for a model with species `A`. More below.

All four of the positional arguments are optional. If any of the positional arguments are a list of string instead of a number, then they are interpreted as a list of selections.

There are a number of ways to call simulate.

1: With no arguments. In this case, the current set of options from the previous `simulate` call will be used. If this is the first time `simulate` is called, then a default set of values is used. The default set of values are (start = 0, end = 5, points = 51).

2: With up to four positions arguments, described above.

Finally, you can pass steps keyword argument instead of points.

steps (Optional) Number of steps at which the output is sampled where the samples are evenly spaced. Steps = points-1. Steps and points may not both be specified.

Returns a numpy array with each selected output time series being a column vector, and the 0'th column is the simulation time.

Return type numpy.ndarray

`RoadRunner.`**`gillespie`**(*start*, *end*, *steps*)

Run a Gillespie stochastic simulation.

Use *`RoadRunner.reset()`* to reset the model each time.

Parameters

- **`start`** – start time
- **`end`** – end time
- **`steps`** – number of steps

Returns a numpy array with each selected output time series being a column vector, and the 0'th column is the simulation time.

Return type numpy.ndarray

Examples:

Simulate from time zero to 40 time units

```
>>> result = r.gillespie (0, 40)
```

Simulate on a grid with 10 points from start 0 to end time 40

```
>>> result = r.gillespie (0, 40, 10)
```

Simulate from time zero to 40 time units using the given selection list

```
>>> result = r.gillespie (0, 40, ['time', 'S1'])
```

Simulate from time zero to 40 time units, on a grid with 20 points using the given selection list

```
>>> result = r.gillespie (0, 40, 20, ['time', 'S1'])
```

RoadRunner.**plot**(*result=None*, *loc='upper left'*, *show=True*)

Plot results from a simulation carried out by the simulate or gillespie functions.

To plot data currently held by roadrunner that was generated in the last simulation, use:

```
>>> r.plot()
```

If you are using Tellurium, see tellurium.ExtendedRoadRunner.plot which supports extra arguements.

Parameters

- **result** (*numpy.ndarray*) – Data returned from a simulate or gillespie call
- **loc** (*str*) – string representing the location of legend i.e. "upper right"

Roadrunner.**getSimulationData**()

Returns the array of simulated data. When simulation has not been run, the function will return an empty array.

Steady State

class RoadRunner.**SteadyStateSolver**

RoadRunner.SteadyStateSolver class.

RoadRunner.**steadyStateSelections**

A list of SelectionRecords which determine what values are used for a steady state calculation. This list may be set by assigning a list of valid selection symbols:

```
>>> r.steadyStateSelections = ['S1', '[S2]', 'P1']
>>> r.steadyStateSelections
['S1', '[S2]', 'P1']
```

RoadRunner.**steadyState**()

Attempts to evaluate the steady state for the model. The method returns a value that indicates how close the solution is to the steady state. The smaller the value the better. Values less than 1E-6 usually indicate a steady state has been found. If necessary the method can be called a second time to improve the solution.

Returns the sum of squares of the steady state solution.

Return type double

RoadRunner.**getSteadyStateValues**()

Performs a steady state calculation (evolves the system to a steady state), then calculates and returns the set of values specified by the steady state selections.

Returns a numpy array corresponding to the values specified by steadyStateSelections

Return type numpy.ndarray

RoadRunner.**getSteadyStateValuesNamedArray**()
Performs a steady state calculation (evolves the system to a steady state), then calculates and returns the set of values specified by the steady state selections with all necessary labels.

Returns a NamedArray corresponding to the values specified by steadyStateSelections

Return type NamedArray

RoadRunner.**getSteadyStateSolver**()
Returns the steady state solver which is currently being used.

RoadRunner.**steadyStateSolverExists**(*name*)
Checks whether a steady state solver exists.

Parameters **name** (*str*) – name of a steady state solver

Metabolic control analysis

In the special case when an SBML model is a purely reaction kinetics model – no rate rules, no assignment rules for chemical species, and time invariant stoichiometry, specialized analysis methods related to metabolic control analysis are applicable. These methods are described in this section.

RoadRunner.**getCC**(*variable*, *parameter*)
Returns a scaled control coefficient with respect to a global parameter.

For example:

```
rr.getCC ('J1', 'Vmax')
rr.getCC ('S1', 'Xo')
rr.getCC ('S2', 'Km')
```

The first returns a flux control coefficient with respect to flux J1. The second and third return concentration control coefficients with respect to species S1 and S2.

Parameters

- **variable** – The id of a dependent variable of the coefficient, for example a reaction or species concentration.
- **parameter** – The id of the independent parameter, for example a kinetic constant or boundary species

Returns the value of the scaled control coefficient.

Return type double

RoadRunner.**getuCC**(*variableId*, *parameterId*)
Get unscaled control coefficient with respect to a global parameter.

Parameters

- **variableId** – The id of a dependent variable of the coefficient, for example a reaction or species concentration.
- **parameterId** – The id of the independent parameter, for example a kinetic constant or boundary species

Returns the value of the unscaled control coefficient.

Return type double

RoadRunner.**getEE**(*reactionId*, *parameterId*, *steadyState=True*)
Retrieve a single elasticity coefficient with respect to a global parameter.

For example:

```
x = rr.getEE ('J1', 'Vmax')
```

calculates elasticity coefficient of reaction 'J1' with restpect to parameter 'Vmax'.

Parameters

- **variable** (*str*) – A reaction Id
- **parameter** (*str*) – The independent parameter, for example a kinetic constant, floating or boundary species
- **steadyState** (*Boolean*) – should the steady state value be computed.

RoadRunner.**getuEE**(*reactionId*, *parameterId*)
Get unscaled elasticity coefficient with respect to a global parameter or species.

RoadRunner.**getEigenValueIds**()
Returns a list of selection symbols for the eigenvalues of the floating species. The eigen value selection symbol is `eigen(XX)`, where `XX` is the floating species name.

RoadRunner.**getFullEigenValues**()
Calculates the eigen values of the Full Jacobian as a real matrix, first column real part, second column imaginary part.

Note, only valid for pure reaction kinetics models (no rate rules, no floating species rules and time invariant stoichiometry).

Return type numpy.ndarray

RoadRunner.**getReducedEigenValues**()
Calculates the eigen values of the Reduced Jacobian as a real matrix, first column real part, second column imaginary part.

Only valid if moiety conversion is enabled.

Note, only valid for pure reaction kinetics models (no rate rules, no floating species rules and time invariant stoichiometry).

Return type numpy.ndarray

RoadRunner.**getFullJacobian**()
Compute the full Jacobian at the current operating point.

This is the Jacobian of ONLY the floating species.

RoadRunner.**getReducedJacobian**()
Returns the *reduced* Jacobian for the independent species. This matrix will be non-singular for models that include moiety-conserved cycles.

Return type numpy.ndarray

RoadRunner.**getScaledConcentrationControlCoefficientMatrix**()
Returns the m by n matrix of scaled concentration control coefficients where m is the number of floating species and n the number of reactions.

Return type numpy.ndarray

RoadRunner.**getScaledFloatingSpeciesElasticity**(*reactionId*, *speciesId*)
Returns the scaled elasticity for a given reaction and given species.

Parameters

- **reactionId** (*str*) – the SBML id of a reaction.
- **speciesId** (*str*) – the SBML id of a species.

Return type double

RoadRunner.**getUnscaledParameterElasticity**(*reactionId*, *parameterId*)
Returns the unscaled elasticity for a named reaction with respect to a named parameter

Parameters

- **reactionId** (*str*) – the SBML id of a reaction.
- **parameterId** (*str*) – the SBML id of a parameter.

Return type double

RoadRunner.**getUnscaledConcentrationControlCoefficientMatrix**()
Returns the unscaled concentration control coefficient matrix.

RoadRunner.**getUnscaledElasticityMatrix**()
Returns the unscaled species elasticity matrix at the current operating point.

RoadRunner.**getUnscaledFluxControlCoefficientMatrix**()
Returns the unscaled flux control coefficient matrix.

RoadRunner.**getUnscaledSpeciesElasticity**(*reactionIndx*, *speciesIndx*)
Get a single species elasticity value.

Parameters

- **reactionIndx** (*int*) – index of reaction
- **speciesIndx** (*int*) – index of species.

RoadRunner.**getScaledFluxControlCoefficientMatrix**()
Returns the n by n matrix of scaled flux control coefficients where n is the number of reactions.

Return type numpy.ndarray

RoadRunner.**getScaledElasticityMatrix**()
Returns the scaled elasticity matrix at the current operating point.

Return type numpy.ndarray

RoadRunner.**getDiffStepSize**()
Returns the differential step size used in routines such as *getCC()*.

RoadRunner.**setDiffStepSize**(*val*)
Sets the differential step size used in routines such as *getCC()*.

Parameters **val** – differential step size

RoadRunner.**getSteadyStateThreshold**()
Returns the threshold used in steady state solver in routines such as *getCC()*.

RoadRunner.**setSteadyStateThreshold**(*val*)
Sets the threshold used in steady state solver in routines such as *getCC()*.

Parameters **val** – threshold value

Stoichiometric Analysis

RoadRunner.**getFullStoichiometryMatrix**()
Get the stoichiometry matrix that coresponds to the full model, even it it was converted via conservation conversion.

RoadRunner.**getReducedStoichiometryMatrix**()
Get the reduced stochiometry matrix. If conservation conversion is enabled, this is the matrix that coresponds to the independent species.

A synonym for getNrMatrix().

RoadRunner.**getConservationMatrix**()
Returns a conservation matrix Γ which is a $c \times m$ matrix where c is the number of conservation laws and m the number of species.

RoadRunner.**getL0Matrix**()
Returns the L0 matrix for the current model. The L0 matrix is an (m-r) by r matrix that expresses the dependent reaction rates in terms of the independent rates. m is the number of floating species and r is the rank of the stoichiometry matrix.

Return type numpy.ndarray

RoadRunner.**getLinkMatrix**()
Returns the full link matrix, L for the current model. The Link matrix is an m by r matrix where m is the number of floating species and r the rank of the stoichiometric matrix, N.

Return type numpy.ndarray

RoadRunner.**getNrMatrix**()
Returns the reduced stoichiometry matrix, N_R, which will have only r rows where r is the rank of the full stoichiometry matrix. The matrix will be reordered such that the rows of N_R are independent.

Return type numpy.ndarray

RoadRunner.**getKMatrix**()
Returns the K matrix, $ker(N_R)$, (right nullspace of Nr) The K matrix has the structure, $[IK0]'$

Return type numpy.ndarray

Analysis

RoadRunner.**getFrequencyResponse**(*startFrequency*, *numberOfDecades*, *numberOfPoints*, *parameterName*, *variableName*, *useDB*, *useHz*)
Computes the frequency response. Returns a numpy array with three columns. First column is the frequency, second column the amplitude, and the third column the phase.

Parameters

- **startFrequency** – Start frequency for the first column in the output
- **numberOfDecades** (*int*) – Number of decades for the frequency range, eg 4 means the frequency span 10,000
- **numberOfPoints** (*int*) – The number of points to generate in the output
- **parameterName** (*str*) – The parameter where the input frequency is applied, usually a boundary species, eg 'Xo'
- **variableName** (*str*) – The amplitude and phase will be output for this variable, usually a floating species, eg 'S1'

- **useDB** (*boolean*) – If true use Decibels on the amplitude axis
- **useHz** (*boolean*) – If true use Hertz on the x axis, the default is rads/sec

For example:

```
import tellurium as te
import roadrunner
from matplotlib import pyplot as plt

r = te.loada("""
    $Xo -> x1; k1*Xo - k2*x1;
     x1 -> x2; k2*x1 - k3*x2;
     x2 ->; k3*x2;

     k1 = 0.5; k2 = 0.23; k3 = 0.4;  Xo = 5;
""")

r.steadyState()

m = r.getFrequencyResponse(0.001, 5, 1000, 'Xo', 'x2', True, False)

fig = plt.figure(figsize=(10,4))

ax1 = fig.add_subplot (121)
ax1.semilogx (m[:,0], m[:,1], color="blue", linewidth="2")
ax1.set_title ('Amplitude')
plt.xlabel ('Frequency')

ax2 = fig.add_subplot (122)
ax2.semilogx (m[:,0], m[:,2], color="blue", linewidth="2")
ax2.set_title ('Phase')
plt.xlabel ('Frequency')
plt.show()
```

RoadRunner.**getRatesOfChange**()

Returns the rates of change of all floating species. The order of species is given by the order of Ids returned by getFloatingSpeciesIds()

Returns a named array of floating species rates of change.

Return type numpy.ndarray

```
>>> r.getRatesOfChange()
         MKKK,       MKKK_P,       MKK,       MKK_P,     MKK_PP,      MAPK,    MAPK_P,
↪  MAPK_PP
[[ 0.000503289, -0.000503289, 0.537508, -0.0994839, -0.438024, 0.061993, 0.108417,
↪ -0.17041]]
```

RoadRunner.**getIndependentRatesOfChange**()

Returns the rates of change of all independent floating species. The order of species is given by the order of Ids returned by getIndependentFloatingSpeciesIds()

Returns a named array of independent floating species rates of change.

Return type numpy.ndarray

```
>>> r.getIndependentRatesOfChange()
        MKK_P,    MAPK_P,         MKKK,       MKK,      MAPK
[[ -0.0994839, 0.108417, 0.000503289, 0.537508, 0.061993]]
```

RoadRunner.**getDependentRatesOfChange**()
Returns the rates of change of all dependent floating species. The order of species is given by the order of Ids returned by getDependentFloatingSpeciesIds()

Returns a named array of dependent floating species rates of change.

Return type numpy.ndarray

```
>>> r.getDependentRatesOfChange()
      MKK_PP,       MKKK_P,   MAPK_PP
[[ -0.438024, -0.000503289, -0.17041]]
```

1.13.3 Solver Class

class roadrunner.**Solver**
Following functions are supported for a given solver instance which can be obtained by calling RoadRunner.getIntegrator() or RoadRunner.getSteadyStateSolver() methods. There are two types of solvers: Integrators(cvode, gillespie, rk4, rk45) - RoadRunner.Integrator() and Steady State Solvers(nleq2) - RoadRunner.SteadyStateSolver()

Solver.**getDescription**(*key*)
If key = None, returns description of this solver. Else, returns the description associated with a given key.

Parameters **key** (*str*) – settings name

Solver.**getDisplayName**(*key*)
Returns display name of given key.

Parameters **key** (*str*) – settings name

Solver.**getHint**(*key*)
If key = None, returns a (user-readable) hint for this solver. Else, Returns the hint associated with a given key.

Parameters **key** (*str*) – settings name

Solver.**getName**()
Returns the name of this solver

Solver.**getNumParams**()
Get the number of parameters.

Solver.**getParamDesc**(*n*)
Get the description of the parameter at index n

Parameters **n** (*int*) – index of parameter

Solver.**getParamDisplayName**(*n*)
Get the display name of the parameter at index n

Parameters **n** (*int*) – index of parameter

Solver.**getParamHint**(*n*)
Get the hint of the parameter at index n.

Parameters **n** (*int*) – index of parameter

Solver.**getParamName**(*n*)
Get the display name of the parameter at index n.

Parameters **n** (*int*) – index of parameter

Solver.**getSetting**(*k*)
Get value of a solver setting

Parameters **k** (*str*) – settings name

Solver.**getSettings**()
Returns a list of all settings for this solver.

Solver.**getSettingsRepr**()
Returns the solver settings as a string.

Solver.**getType**(*key*)
Returns the type associated with a given key.

Parameters **key** (*str*) – settings name

Solver.**getValue**(*key*)
Get the value of an integrator setting.

Parameters **key** (*str*) – settings name

Solver.**getValueAsBool**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsChar**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsDouble**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsFloat**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsInt**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsLong**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsString**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsUChar**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsUInt**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**getValueAsULong**(*key*)
Wrapper for *Solver.getValue()* which converts output to a specific type

Parameters **key** (*str*) – settings name

Solver.**hasValue**(*key*)
Return true if this setting is supported by the integrator.

Parameters **key** (*str*) – settings name

Solver.**resetSettings**()
Reset all settings to their respective default values.

Solver.**setSetting**(*k*, *v*)
Set value of a solver setting

Parameters

- **k** (*str*) – settings name
- **v** (*const*) – value of the setting

Solver.**setValue**(*key*, *value*)
Sets value of a specific setting.

Parameters

- **key** (*str*) – settings name
- **value** (*const*) – value of the setting

Solver.**settingsPyDictRepr**()
Returns Python dictionary-style string representation of settings.

Solver.**syncWithModel**(*m*)
Called whenever a new model is loaded to allow integrator to reset internal state

Parameters **m** (*object*) – new model

Solver.**toRepr**()
Return string representation a la Python __repr__ method.

Solver.**toString**()
Return a string representation of the solver.

1.13.4 Integrator Class

class roadrunner.**Integrator**
An integrator is used to describe the method of carrying out a mathematical integration. Currently, libRoadRunner supports cvode, gillespie, rk4 and rk45 solvers. For solver related methods, refer to http://sys-bio.github.io/roadrunner/python_docs/api_reference.html#solver-class. The following methods are supported by all the Integrators.

Integrator.**getIntegrationMethod**()
Gets the method of integration as an integer. (0-Deterministic, 1-Stochastic, 2-Hybrid, 3-Other).

Integrator.**getListener**()
Gets the integrator listener.

Integrator.**integrate**(*t0*, *hstep*)
Main integration routine.

Parameters

- **t0** (*double*) – start time
- **hstep** (*double*) – time step size

Integrator.**loadSBMLSettings**(*filename*)
Load an SBML settings file and apply the configuration options. Note: Can assign relative and absolute tolerances.

Parameters **filename** (*string*) – A string which may be a local path, URI or contents of an SBML document.

Integrator.**restart**(*t0*)
Reset time to zero and reinitialize model. Applies events which occur before time zero. Reinitializes CVODE and the executable model.

Parameters **t0** (*double*) – start time

Integrator.**setListener**(*listener*)
Sets the integrator listener.

Parameters **listener** – Swig Object of type 'rr::PyIntegratorListenerPtr *'

Integrator.**tweakTolerances**()
Fix tolerances for SBML tests. In order to ensure that the results of the SBML test suite remain valid, this method enforces a lower bound on tolerance values. Sets minimum absolute and relative tolerances to Config::CVODE_MIN_ABSOLUTE and Config::CVODE_MIN_RELATIVE respectively.

Integrator.**setIndividualTolerance**(*sid*, *value*)
Sets absolute tolerance for individual floating species or variable that has a rate rule. Only used for CVODE Integrator. Note that this tolerance is based on the amount of species, and will be stored in absolute_tolerance.

Parameters

- **sid** (*str*) – identifier of individual species or varible that has a rate rule
- **value** (*double*) – tolerance value to set

Integrator.**setConcentrationTolerance**(*value*)
Sets the tolerance based on concentration of species. Only used for CVODE Integrator. First converts the concentration tolerances to amount tolerances by multiplying the compartment volume of species. Whichever is smaller will be stored in absolute_tolerance and used in the integration process. Note that if a double list is given, the size of list must be equal to numIndFloatingSpecies+numRateRule, including tolerances for each independent floating species that doesn't have a rate rule followed by tolerances for each variable(including dependent floating species) that has a rate rule. The order of independent floating species and variables is the same as the order how they were defined in species list and rate rule list.

Parameters **list value** (*double/double*) – tolerance value to set

Integrator.**getConcentrationTolerance**()
Gets the tolerance vector based on concentration of species. Only used for CVODE Integrator. The vector includes tolerances for each independent floating species that doesn't have a rate rule followed by tolerances for each variable(including dependent floating species) that has a rate rule. The order of independent floating species and variables is the same as the order how they were defined in species list and rate rule list.

CVODE

CVODE is a deterministic ODE solver from the SUNDIALS suite of timecourse integrators. It implements an Adams-Moulton solver for non-stiff problems and a backward differentiation formula (BDF) solver for stiff problems.

Integrator.**absolute_tolerance**
Specifies the scalar or vector absolute tolerance based on amount of species. A potentially different absolute tolerance for each vector component could be set using a double vector. CVODE then calculates a vector of error

weights which is used in all error and convergence tests. The weighted RMS norm for the absolute tolerance should not become smaller than this value. Default value is Config::CVODE_MIN_ABSOLUTE.

```
>>> r.integrator.absolute_tolerance = 1
>>> r.integrator.absolute_tolerance = [1, 0.1, 0.01, 0.001] // setting vairous␣
↪tolerance for each species
```

Integrator.**initial_time_step**
Specifies the initial time step size. If inappropriate, CVODE will attempt to estimate a better initial time step. Default value is 0.0

```
>>> r.integrator.initial_time_step = 1
```

Integrator.**maximum_adams_order**
Specifies the maximum order for Adams-Moulton intergration. This integration method is used for non-stiff problems. Default value is 12.

```
>>> r.integrator.maximum_adams_order = 20
```

Integrator.**maximum_bdf_order**
Specifies the maximum order for Backward Differentiation Formula integration. This integration method is used for stiff problems. Default value is 5.

Integrator.**maximum_num_steps**
Specifies the maximum number of steps to be taken by the CVODE solver in its attempt to reach tout. Default value is 20000.

Integrator.**maximum_time_step**
Specifies the maximum absolute value of step size allowed. If inappropriate, CVODE will attempt to estimate a better maximum time step. Default value is 0.0.

Integrator.**minimum_time_step**
Specifies the minimum absolute value of step size allowed. If inappropriate, CVODE will attempt to estimate a better maximum time step. Default value is 0.0.

Integrator.**multiple_steps**
Perform a multiple time step simulation. Default value is false.

```
>>> r.integrator.multiple_steps = True
```

Integrator.**relative_tolerance**
Specifies the scalar relative tolerance. CVODE calculates a vector of error weights which is used in all error and convergence tests. The weighted RMS norm for the relative tolerance should not become smaller than this value. Default value is Config::CVODE_MIN_RELATIVE.

Integrator.**stiff**
Specifies whether the integrator attempts to solve stiff equations. Ensure the integrator can solver stiff differential equations by setting this value to true. Default value is true.

Integrator.**variable_step_size**
Perform a variable time step simulation. Enabling this setting will allow the integrator to adapt the size of each time step. This will result in a non-uniform time column. Default value is flase.

Gillespie

RoadRunner's implementation of the standard Gillespie Direct Method SSA. The granularity of this simulator is individual molecules and kinetic processes are stochastic. Results will, in general, be different in each run, but a sufficiently large ensemble of runs should be statistically correct.

Can be used with the r.gillespie function or by setting integrator to gillespie (see below)

`Integrator.`**`initial_time_step`**
Specifies the initial time step size. If inappropriate, CVODE will attempt to estimate a better initial time step. Default value is 0.0

```
>>> r.setIntegrator('gillespie') # set integrator first
>>> r.integrator.initial_time_step = 2
```

`Integrator.`**`maximum_time_step`**
Specifies the maximum absolute value of step size allowed. If inappropriate, CVODE will attempt to estimate a better maximum time step. Default value is 0.0.

`Integrator.`**`minimum_time_step`**
Specifies the minimum absolute value of step size allowed. If inappropriate, CVODE will attempt to estimate a better maximum time step. Default value is 0.0.

`Integrator.`**`nonnegative`**
Prevents species amounts from going negative during a simulation. Default value is false.

`Integrator.`**`seed`**
Set the seed into the random engine.

`Integrator.`**`variable_step_size`**
Perform a variable time step simulation. Enabling this setting will allow the integrator to adapt the size of each time step. This will result in a non-uniform time column. Default value is flase.

Euler

The Euler method is one of the simplest approaches to solving a first order ODE. Given the rate of change of function f at time t, it computes the new value of f as `f(t+h) = f(t) + h*f'(t)`, where h is the time step. Euler's method is rarely used in practice due to poor numerical robustness. Can be used with:

```
>>> r.setIntegrator('euler')
```

RK4

Runge-Kutta methods are a family of algorithms for solving ODEs. They have considerably better accuracy than the Euler method. This integrator is a standard 4th order Runge-Kutta solver. Can be used with:

```
>>> r.setIntegrator('rk4')
```

RK45

RoadRunner's implementation of the standard Gillespie Direct Method SSA. The granularity of this simulator is individual molecules and kinetic processes are stochastic. Results will, in general, be different in each run, but a sufficiently large ensemble of runs should be statistically correct.

`Integrator.`**`epsilon`**
Specifies the maximum error tolerance allowed. Default value is 1e-12.

```
>>> r.setIntegrator('rk45') # set integrator first
>>> r.integrator.epsilon = 1e-10
```

Integrator.**maximum_time_step**
Specifies the maximum absolute value of step size allowed. If inappropriate, CVODE will attempt to estimate a better maximum time step. Default value is 0.0.

Integrator.**minimum_time_step**
Specifies the minimum absolute value of step size allowed. If inappropriate, CVODE will attempt to estimate a better maximum time step. Default value is 0.0.

Integrator.**variable_step_size**
Perform a variable time step simulation. Enabling this setting will allow the integrator to adapt the size of each time step. This will result in a non-uniform time column. Default value is flase.

1.13.5 Steady State Solver Class

class roadrunner.**SteadyStateSolver**
A Steady State Solver gives the steady states of involved species. Currently, libRoadRunner supports NLEQ2 solver. For solver related methods, refer to http://sys-bio.github.io/roadrunner/python_docs/api_reference.html#solver-class.

NLEQ2

NLEQ2 is a non-linear equation solver which uses a global Newton method with adaptive damping strategies (see http://www.zib.de/weimann/NewtonLib/index.html).

SteadyStateSolver.**allow_presimulation**
Flag for starting steady state analysis with simulation. This flag does not affect the usage of approximation routine when the default steaty state solver fails. Default value is false.

To enable, type:

```
>>> r.getSteadyStateSolver().allow_presimulation = True
```

SteadyStateSolver.**presimulation_tolerance**
Tolerance for presimulation before steady state analysis. Absolute tolerance used by presimulation routine. Only used when allow_presimulation is True. Default value is 1e-3.

```
>>> r.getSteadyStateSolver().presimulation_tolerance = 1e-2
```

SteadyStateSolver.**presimulation_maximum_steps**
Maximum number of steps that can be taken for presimulation before steady state analysis. Takes priority over presimulation_time. Only used when allow_presimulation is True. Default value is 100.

```
>>> r.getSteadyStateSolver().presimulation_maximum_steps = 50
```

SteadyStateSolver.**presimulation_time**
End time for presimulation steady state analysis. Only used when allow_presimulation is True. Default value is 100.

```
>>> r.getSteadyStateSolver().presimulation_time = 50
```

SteadyStateSolver.**allow_approx**
Flag for using steady state approximation routine when steady state solver fails. Approximation routine will run only when the default solver fails to fine a solution. This flag does not affect usage of approximation routine for pre-simulation. Default is True.

To disable, type:

```
>>> r.getSteadyStateSolver().allow_approx = False
```

SteadyStateSolver.**approx_tolerance**
Tolerance for steady state approximation routine. Absolute tolerance used by steady state approximation routine. Only used when steady state approximation routine is used. Default value is 1e-12.

```
>>> r.getSteadyStateSolver().approx_tolerance = 1e-6
```

SteadyStateSolver.**approx_maximum_steps**
Maximum number of steps that can be taken for steady state approximation routine. Takes priority over approx_time. Only used when steady state approximation routine is used. Default value is 10000.

```
>>> r.getSteadyStateSolver().approx_maximum_steps = 5000
```

SteadyStateSolver.**approx_time**
End time for steady state approximation routine. approx_maximum_steps takes priority. Only used when steady state approximation routine is used. Default value is 10000.

```
>>> r.getSteadyStateSolver().approx_time = 5000
```

SteadyStateSolver.**broyden_method**

Switches on Broyden method, which is a quasi-Newton approximation for rank-1 updates. Default value is 0.

To enable, type:

```
>>> r.getSteadyStateSolver().broyden_method = 1
```

SteadyStateSolver.**linearity**
Specifies linearity of the problem. 1 is for linear problem and 4 is for extremly nonlinear problem. Default value is 3.

```
>>> r.getSteadyStateSolver().linearity = 1
```

SteadyStateSolver.**maximum_iterations**
The maximum number of iterations the solver is allowed to use. Iteration caps off at the maximum, regardless of whether a solution has been reached. Default value is 100.

```
>>> r.getSteadyStateSolver().maximum_iterations = 50
```

SteadyStateSolver.**minimum_damping**
The minimum damping factor used by the algorithm. Default value is 1e-4.

```
>>> r.getSteadyStateSolver().minimum_damping = 1e-20
```

SteadyStateSolver.**relative_tolerance**
Specifies the relative tolerance used by the solver. Default value is 1e-16.

```
>>> r.getSteadyStateSolver().relative_tolerance = 1e-15
```

SteadyStateSolver.**solve**()
Main solver routine

1.13.6 SelectionRecord

class roadrunner.**SelectionRecord**(*str*)

RoadRunner provides a range of flexible ways of selecting values from a simulation. These values can not only be calculated directly via RoadRunner.getSelectionValue, but any of these selections can be used as columns in the simulate result matrix.

The SectionRecord.selectionType should be one of the constants listed here.

p1 and p2 may be required along with the attribute to set certain selection types that use one or more arguments.

Below is the list of attributes which are FOR ADVANCED USERS ONLY. For simplified usage, refer to *Selecting Values*.

SelectionRecord.**ALL**

SelectionRecord.**ALL_DEPENDENT**

SelectionRecord.**ALL_DEPENDENT_AMOUNT**

SelectionRecord.**ALL_DEPENDENT_CONCENTRATION**

SelectionRecord.**ALL_INDEPENDENT**

SelectionRecord.**ALL_INDEPENDENT_AMOUNT**

SelectionRecord.**ALL_INDEPENDENT_CONCENTRATION**

SelectionRecord.**AMOUNT**
species must have either a CONCENTRATION or AMOUNT modifer to distinguish it.

SelectionRecord.**BOUNDARY**
species must have either a BOUNDARY or FLOATING modifiers.

SelectionRecord.**BOUNDARY_AMOUNT**
boundary species amount

SelectionRecord.**BOUNDARY_CONCENTRATION**
boundary species concentration

SelectionRecord.**_COMPARTMENT**
Compartments and parameters can be either current or initial values. These values with and underscore, '_' are intended to be used with either an CURRENT or INITIAL value modifier.

SelectionRecord.**COMPARTMENT**
the current compartment value

SelectionRecord.**CONCENTRATION**
species must have either a CONCENTRATION or AMOUNT modifer to distinguish it.

SelectionRecord.**CONSREVED_MOIETY**

SelectionRecord.**CONTROL**
scaled control coefficient of designated arguments.

SelectionRecord.**CURRENT**

SelectionRecord.**DEPENDENT**

SelectionRecord.**EIGENVALUE**
real part of eigenvalue of designated identifier.

SelectionRecord.**EIGENVALUE_COMPLEX**
complex part of eigenvalue of designated identifier.

SelectionRecord.**ELASTICITY**
scaled elasticity coefficient of designated arguments.

SelectionRecord.**ELEMENT**

SelectionRecord.**FLOATING**
species must have either a BOUNDARY or FLOATING modifiers.

SelectionRecord.**FLOATING_AMOUNT**
floating species current amounts.

SelectionRecord.**FLOATING_AMOUNT_RATE**
floating species amount rates (value, not reaction rates)

SelectionRecord.**FLOATING_CONCENTRATION**
floating species current concentrations.

SelectionRecord.**FLOATING_CONCENTRATION_RATE**

SelectionRecord.**GLOBAL_PARAMETER**
the current global parameter value

SelectionRecord.**INDEPENDENT**

SelectionRecord.**INITIAL**

SelectionRecord.**INITIAL_FLOATING_AMOUNT**
initial amount of designated identifier.

SelectionRecord.**INITIAL_FLOATING_CONCENTRATION**
initial concentration of designated identifier.

SelectionRecord.**RATE**

SelectionRecord.**REACTION**

SelectionRecord.**REACTION_RATE**
current reaction rate

SelectionRecord.**STOICHIOMETRY**
stoichiometric coefficient of designated identifier and reaction.

SelectionRecord.**TIME**

SelectionRecord.**UNKNOWN**

SelectionRecord.**UNKNOWN_CONCENTRATION**

SelectionRecord.**UNKNOWN_ELEMENT**

SelectionRecord.**UNSCALED**

SelectionRecord.**UNSCALED_CONTROL**
unscaled control coefficient of designated arguments.

SelectionRecord.**UNSCALED_ELASTICITY**
unscaled elasticity coefficient of designated arguments.

SelectionRecord.**index int**

SelectionRecord.**p1 str**
first of the arguments

SelectionRecord.**p2 str**
second of the arguments

SelectionRecord.**selectionType int**

1.13.7 SBML Compile Options

class RoadRunner.**LoadSBMLOptions**
The LoadSBMLOptions object allows tuning a variety of SBML loading and compilations options.

This object can be passed in as the second, optional argument of the `RoadRunner.__init__()` constructor, or the *RoadRunner.load()* method.

LoadSBMLOptions.**conservedMoieties bool**
Performs conservation analysis.

This causes a re-ordering of the species, so results generated with this flag enabled can not be compared index wise to results generated otherwise.

Moiety conservation is only compatable with simple models which do NOT have any events or rules which define or alter any floating species, and which have simple constant stiochiometries.

LoadSBMLOptions.**mutableInitialConditions bool**
Generates accessor functions to allow changing of initial conditions.

LoadSBMLOptions.**noDefaultSelections bool**
If True, do not create a default selection list when the model is loaded.

LoadSBMLOptions.**readOnly bool**
Should the model be recompiled? The LLVM ModelGenerator maintains a hash table of currently running models. If this flag is NOT set, then the generator will look to see if there is already a running instance of the given model and use the generated code from that one.

If only a single instance of a model is run, there is no need to cache the models, and this can safely be enabled, realizing some performance gains.

LoadSBMLOptions.**recompile bool**
If this is set, then a read-only model is generated. A read-only model can be simulated, but no code is generated to set model values, i.e. parameters, amounts, values, etc...

It takes a finite amount of time to generate the model value setting functions, and if they are not needed, one may see some performance gains, especially in very large models.

1.13.8 Accessing the SBML Model Variables

All of the SBML model variables are accessed via the `RoadRunner.model` object. This is an instance of the ExecutableModel class described here. One always access the model object that belongs to the top RoadRunner object, i.e. `r.model`, where `r` is an instance of the `RoadRunner` class.

The ExecutableModel class also implements the Python dictionary protocol, so that it can be used as a dictionary. The dictionary keys are all of the symbols specified in the original model as well as a number of selection strings described in the Selections section.

ExecutableModel.**keys**()
Get a list of all the keys that this model has. This is a very good way of looking at all the available symbols and selection strings:

```
>>> r.model.keys()
[ 'S1', 'S2', '[S1]', '[S2]', 'compartment', 'k1', 'cm0',
  'reaction1',  'init([S1])',  'init([S2])', 'init(S1)',
  'init(S2)',  "S1'"]
```

ExecutableModel.**items**()
Get a list of key / value pairs of all the selections / values in the model.

```
>>> r.model.items()
[('S1', 0.5), ('S2', 9.99954570660308), ('[S1]', 0.5), ('[S2]', 9.99954570660308),
('default_compartment', 1.0), ('k1', 1.0), ('init(k1)', 1.0), ('_J0', 0.5), (
↪'init([S1])', 10.0),
('init([S2])', 0.0), ('init(S1)', 10.0), ('init(S2)', 0.0), ("S1'", -0.5), ("S2'",
↪ 0.5)]
```

ExecutableModel.**__getitem__**()
Implements the python [] indexing operator, so the model values can be accessed like:

```
>>> r.model["S1"]
0.0
```

Following notation is also accepted:

```
>>> r.S1
0.0
```

ExecutableModel.**__setitem__**()
Implements the python [] indexing operator for setting values:

```
>>> r.model["S1]
0.0
>>> r.model["S1"] = 1.3
>>> r.model["S1"]
1.3
```

Following notation is also accepted:

```
>>> r.S1 = 1.0
```

Note, some keys are read only such as values defined by rules, or calculated values such as reaction rates. If one attempts to set the value of a read-only symbol, an exception is raised indicating the error, and no harm done.

Floating Species

ExecutableModel.**getFloatingSpeciesIds**()
Return a list of all floating species SBML ids.

```
>>> r.getFloatingSpeciesIds()
['S1', 'S2', 'S3', 'S4']
```

ExecutableModel.**getDependentFloatingSpeciesIds**()
Return a list of dependent floating species SBML ids.

```
>>> r.getDependentFloatingSpeciesIds()
['S4']
```

ExecutableModel.**getIndependentFloatingSpeciesIds**()
Return a list of independent floating species SBML ids.

```
>>> r.getIndependentFloatingSpeciesIds()
['S1', 'S2', 'S3']
```

ExecutableModel.**getFloatingSpeciesConcentrationIds**()
Return a list of all floating species concentration ids.

```
>>> r.getFloatingSpeciesConcentrationIds()
['[S1]', '[S2]', '[S3]', '[S4]']
```

ExecutableModel.**getNumFloatingSpecies**()

Return the number of floating species in the model.

```
>>> r.getNumFloatingSpecies()
2
```

ExecutableModel.**getFloatingSpeciesAmounts**([*index*])

Get the list of floating species amounts. If no arguments are given, this returns all floating species amounts.

Parameters **index** (*numpy.ndarray*) – (optional) an optional array of desired floating species indices.

Retuns an array of floating species amounts.

Return type numpy.ndarray

To get all the amounts:

```
>>> r.model.getFloatingSpeciesAmounts()
array([ 0.97390578,  1.56331018,  1.15301155,  1.22717548])
```

To get amounts from index 0 and 1:

```
>>> r.model.getFloatingSpeciesAmounts([0,1])
array([ 0.97390578,  1.56331018])
```

ExecutableModel.**setFloatingSpeciesAmounts**([*index*], *values*)

Use this to set the entire set of floating species amounts in one call. The order of species is given by the order of Ids returned by getFloatingSpeciesIds()

Parameters

- **index** (*numpy.ndarray*) – (optional) an index array indicating which items to set, or if no index array is given, the first param should be an array of all the values to set.
- **values** (*numpy.ndarray*) – the values to set.

```
>>> r.model.getFloatingSpeciesAmounts([0,1])
array([ 0.97390578,  1.56331018])
>>> r.model.setFloatingSpeciesAmounts([0,1], [1.0, 1.5])
>>> r.model.getFloatingSpeciesAmounts([0,1])
array([ 1. ,  1.5])
```

ExecutableModel.**getFloatingSpeciesConcentrations**([*index*])

Return a vector of floating species concentrations. The order of species is given by the order of Ids returned by getFloatingSpeciesIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of floating species concentrations.

Return type numpy.ndarray

```
>>> r.model.getFloatingSpeciesConcentrations()
array([  4.54293397e-04,   9.99954571e+00])
```

ExecutableModel.**setFloatingSpeciesConcentrations**([*index*], *values*)
Use this to set the entire set of floating species concentrations in one call. The order of species is given by the order of Ids returned by getFloatingSpeciesIds()

Parameters

- **index** (*numpy.ndarray*) – (optional) an index array indicating which items to set, or if no index array is given, the first param should be an array of all the values to set.
- **values** (*numpy.ndarray*) – the values to set.

```
>>> r.model.getFloatingSpeciesConcentrations()
array([  4.54293397e-04,   9.99954571e+00])
>>> r.model.setFloatingSpeciesConcentrations([0],[0.5])
>>> r.model.getFloatingSpeciesConcentrations()
array([ 0.5       ,  9.99954571])
```

Floating Species Initial Conditions

RoadRunner stores all initial conditions separately from the model state variables. This means that you can update the initial conditions at any time, and it does not affect the current state of the model. To reset the model, that is, reset it to its original state, or a new original state where what has changed the initial conditions use the `reset()` method.

The following methods allow access to the floating species initial condition values:

ExecutableModel.**getFloatingSpeciesInitAmountIds**()
Return a list of the floating species amount initial amount selection symbols.

```
>>> r.model.getFloatingSpeciesInitAmountIds()
['init(S1)', 'init(S2)']
```

ExecutableModel.**getFloatingSpeciesInitConcentrationIds**()
Return a list of the floating species amount initial concentration selection symbols.

```
>>> r.model.getFloatingSpeciesInitConcentrationIds()
['init([S1])', 'init([S2])']
```

ExecutableModel.**getFloatingSpeciesInitConcentrations**([*index*])
Return a vector of floating species initial concentrations. The order of species is given by the order of Ids returned by getFloatingSpeciesInitialConcentrationIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of floating species initial concentrations.

Return type numpy.ndarray

```
>>> r.model.getFloatingSpeciesInitConcentrations()
array([ 10.,   0.])
```

ExecutableModel.**setFloatingSpeciesInitConcentrations**([*index*], *values*)
Set a vector of floating species initial concentrations. The order of species is given by the order of Ids returned by getFloatingSpeciesInitialAmountIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

```
>>> r.model.setFloatingSpeciesInitConcentrations([0], [1])
>>> r.model.getFloatingSpeciesInitConcentrations()
array([ 1.,  0.])
```

ExecutableModel.**getFloatingSpeciesInitAmounts**([*index*])

Return a vector of floating species initial amounts. The order of species is given by the order of Ids returned by getFloatingSpeciesInitialConcentrationIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of floating species initial amounts.

Return type numpy.ndarray

```
>>> r.model.getFloatingSpeciesInitAmounts()
array([ 10.,   0.])
```

ExecutableModel.**setFloatingSpeciesInitAmounts**([*index*], *values*)

Set a vector of floating species initial amounts. The order of species is given by the order of Ids returned by getFloatingSpeciesInitialAmountIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

```
>>> r.model.setFloatingSpeciesInitAmounts([0], [0.1])
>>> r.model.getFloatingSpeciesInitAmounts()
array([ 0.1,  0. ])
```

Boundary Species

ExecutableModel.**getBoundarySpeciesAmounts**([*index*])

Return a vector of boundary species amounts. The order of species is given by the order of Ids returned by getBoundarySpeciesIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of the boundary species amounts.

Return type numpy.ndarray

```
>>> r.model.getBoundarySpeciesAmounts()
array([ 15.,   0.])
```

ExecutableModel.**getBoundarySpeciesConcentrations**([*index*])

Return a vector of boundary species concentrations. The order of species is given by the order of Ids returned by getBoundarySpeciesIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of the boundary species concentrations.

Return type numpy.ndarray

```
>>> r.getBoundarySpeciesConcentrations()
array([ 0.5,   0.])
```

ExecutableModel.**getBoundarySpeciesIds**()
Return a vector of boundary species Ids.

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns a list of boundary species ids.

```
>>> r.getBoundarySpeciesIds()
['X0', 'X1']
```

ExecutableModel.**getBoundarySpeciesConcentrationIds**()
Return a vector of boundary species concentration Ids.

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns a list of boundary species concentration ids.

```
>>> r.getBoundarySpeciesConcentrationIds()
['[X0]', '[X1]']
```

ExecutableModel.**getNumBoundarySpecies**()
Return the number of boundary species in the model.

```
>>> r.getNumBoundarySpecies()
2
```

ExecutableModel.**setBoundarySpeciesConcentrations**([*index*], *values*)
Use this to set the entire set of boundary species concentrations in one call. The order of species is given by the order of boundary species returned by getBoundarySpeciesIds()

Parameters

- **index** (*numpy.ndarray*) – (optional) an index array indicating which items to set, or if no index array is given, the first param should be an array of all the values to set.
- **values** (*numpy.ndarray*) – the values to set.

```
>>> r.model.setBoundarySpeciesConcentrations([0], [1])
>>> r.getBoundarySpeciesConcentrations()
array([ 1.,  0.])
```

Compartments

ExecutableModel.**getCompartmentIds**([*index*])
Return a vector of compartment identifier symbols.

Parameters **index** (*None or numpy.ndarray*) – A array of compartment indices indicating which compartment ids to return.

Returns a list of compartment ids.

```
>>> r.getCompartmentIds()
['compartment1']
```

ExecutableModel.**getCompartmentVolumes**([*index*])
Return a vector of compartment volumes. The order of volumes is given by the order of Ids returned by getCompartmentIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of compartment volumes.

Return type numpy.ndarray.

```
>>> r.getCompartmentVolumes()
array([ 1.])
```

ExecutableModel.**getNumCompartments**()

Return the number of compartments in the model.

Return type int

```
>>> r.getNumCompartments()
1
```

ExecutableModel.**setCompartmentVolumes**([*index*], *values*)

Set a vector of compartment volumes.

If the index vector is not give, then the values vector treated as a vector of all compartment volumes to set. If index is given, then values should have the same length as index.

Parameters

- **index** (*numpy.ndarray*) – (optional) an index array indicating which items to set, or if no index array is given, the first param should be an array of all the values to set.
- **values** (*numpy.ndarray*) – the values to set.

```
>>> r.model.setCompartmentVolumes([0], [2.5])
>>> r.getCompartmentVolumes()
array([ 2.5])
```

Global Parameters

ExecutableModel.**getGlobalParameterIds**()

Return a list of global parameter ids.

Returns a list of global parameter ids.

ExecutableModel.**getGlobalParameterValues**([*index*])

Returns a vector of global parameter values. The order of species is given by the order of Ids returned by getGlobalParameterIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of global parameter values.

Return type numpy.ndarray.

```
>>> r.getGlobalParameterValues()
array([ 10. ,  10. ,  10. ,   2.5,   0.5])
```

ExecutableModel.**getNumGlobalParameters**()

Returns the number of global parameters in the model.

```
>>> r.getNumGlobalParameters()
5
```

ExecutableModel.**setGlobalParameterValues**([*index*], *values*)

Sets the entire set of global parameters. The order of parameters is given by the order of Ids returned by getGlobalParameterIds()

Parameters

- **index** (*numpy.ndarray*) – (optional) an index array indicating which items to set, or if no index array is given, the first param should be an array of all the values to set.
- **values** (*numpy.ndarray*) – the values to set.

```
>>> r.model.setGlobalParameterValues([0], [1.5])
>>> r.getGlobalParameterValues()
array([  1.5,  10. ,  10. ,   2.5,   0.5])
```

Reactions

ExecutableModel.**getNumReactions**()

Return the number of reactions in the model.

```
>>> r.getNumReactions()
5
```

ExecutableModel.**getReactionIds**()

Return a vector of reaction Ids.

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns a list of reaction ids.

```
>>> r.getReactionIds()
['J0', 'J1', 'J2', 'J3', 'J4']
```

ExecutableModel.**getReactionRates**([*index*])

Return a vector of reaction rates (reaction velocity) for the current state of the model. The order of reaction rates is given by the order of Ids returned by getReactionIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of reaction rates.

Return type numpy.ndarray

```
>>> r.getReactionRates()
array([ 0.14979613,  2.37711263,  2.68498886,  2.41265507,  1.89417737])
```

Events

ExecutableModel.**getNumEvents**()

Returns the number of events.

```
>>> r.getNumEvents()
1
```

Rate Rules

ExecutableModel.**getNumRateRules**()
Returns the number of rate rules.

```
>>> r.getNumRateRules()
1
```

ExecutableModel.**getEventIds**()
Returns a list of event ids.

Returns a list of event ids.

```
>>> r.model.getEventIds()
['E1']
```

Stoichiometry

ExecutableModel.**getStoichiometry**(*speciesIndex*, *reactionIndex*)
Return the stochiometric coefficient for the given species index and reaction index.

Frequently one does not need the full stochiometrix matrix, particularly if the system is large and only a single coefficient is needed.

Parameters

- **speciesIndex** – a floating species index from *getFloatingSpeciesIds()*
- **reactionIndex** – a reaction index from *getReactionIds()*

```
>>> r.model.getStoichiometry(1, 3)
1.0
```

Conserved Moieties

Refer to RoadRunner.conservedMoietyAnalysis and Config.LOADSBMLOPTIONS_CONSERVED_MOIETIES for more information.

ExecutableModel.**getNumConservedMoieties**()
Return the number of conserved moieties in the model.

Return type int

```
>>> r.getNumConservedMoieties()
1
```

ExecutableModel.**getConservedMoietyIds**([*index*])
Return a vector of conserved moiety identifier symbols.

Parameters **index** (*None or numpy.ndarray*) – A array of compartment indices indicating which compartment ids to return.

Returns a list of compartment ids.

```
>>> r.getConservedMoietyIds()
['_CSUM0']
```

ExecutableModel.**getConservedMoietyValues**([*index*])

Return a vector of conserved moiety volumes. The order of values is given by the order of Ids returned by getConservedMoietyIds()

Parameters **index** (*numpy.ndarray*) – (optional) an index array indicating which items to return.

Returns an array of conserved moiety values.

Return type numpy.ndarray.

```
>>> r.getConservedMoietyValues()
array([ 2.])
```

ExecutableModel.**setConservedMoietyValues**([*index*], *values*)

Set a vector of conserved moiety values.

Note This method currently only updates the conserved moiety values, it does not update the initial species condition from which the values were calculated.

If the index vector is not given, then the values vector treated as a vector of all values to set. If index is given, then values should have the same length as index.

Parameters

- **index** (*numpy.ndarray*) – (optional) an index array indicating which items to set, or if no index array is given, the first param should be an array of all the values to set.
- **values** (*numpy.ndarray*) – the values to set.

```
>>> r.model.setConservedMoietyValues([0], [5])
>>> r.getConservedMoietyValues()
array([ 5.])
```

Misc

ExecutableModel.**getAllTimeCourseComponentIds**()

Return a list of all component ids. The list includes ids of amount/concentration of floating species, boundary species, global parameters, compartments, and reactions, as well as *time*.

Returns a list of all component ids widely used in time course selections.

```
>>> r.model.getAllTimeCourseComponentIds()
['time', 'S1', 'S2', 'S3', 'k1', 'k2', 'default_compartment', '_J0', '_J1']
```

ExecutableModel.**getInfo**()

Get various info about the model.

```
>>> print(r.getInfo())
<roadrunner.RoadRunner() {
'this' : 13DEF5F8
'modelLoaded' : true
'modelName' : feedback
'libSBMLVersion' : LibSBML Version: 5.12.0
'jacobianStepSize' : 1e-005
```

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```
'conservedMoietyAnalysis' : false
'simulateOptions' :
< roadrunner.SimulateOptions()
{
'this' : 0068A7F0,
'reset' : 0,
'structuredResult' : 0,
'copyResult' : 1,
'steps' : 50,
'start' : 0,
'duration' : 40
}>,
'integrator' :
< roadrunner.Integrator() >
  name: cvode
  settings:
      relative_tolerance: 0.00001
      absolute_tolerance: 0.0000000001
                  stiff: true
       maximum_bdf_order: 5
     maximum_adams_order: 12
       maximum_num_steps: 20000
       maximum_time_step: 0
          minimum_time_step: 0
       initial_time_step: 0
          multiple_steps: false
      variable_step_size: false
}>
```

ExecutableModel.**getModelName**()

Get the model name specified in the SBML.

```
>>> r.model.getModelName()
'feedback'
```

ExecutableModel.**getTime**()

Get the model time. The model originally start at time t=0 and is advaced forward in time by the integrator. So, if one ran a simulation from time = 0 to time = 10, the model will then have it's time = 10.

```
>>> r.model.getTime()
40.0
```

ExecutableModel.**setTime**(*time*)

Set the model time variable.

Parameters **time** – time the time value to set.

```
>>> rr.model.setTime(20.)
>>> rr.model.getTime()
20.0
```

ExecutableModel.**reset**()

Resets all the floating species concentrations to their initial values.

ExecutableModel.**resetAll**()

Resets all variables, species, etc. to the CURRENT initial values. It also resets all parameter back to the values they had when the model was first loaded

ExecutableModel.**resetToOrigin**()
Resets the model back to the state is was when it was FIRST loaded. The scope of reset includes all initial values and parameters, etc.

1.13.9 Logging

RoadRunner has extensive logging system. Many internal methods will log extensive details (in full color) to either the clog (typically stderr) or a user specified file path. Internally, the RoadRunner logging system is currently implemented by the Poco (http://pocoproject) logging system.

Future versions will include a Logging Listener, so that the RoadRunner log will log messages to a user specified function.

The logging system is highly configurable, users have complete control over the color and format of the logging messages.

All methods of the Logger are static, they are available immediately upon loading the RoadRunner package.

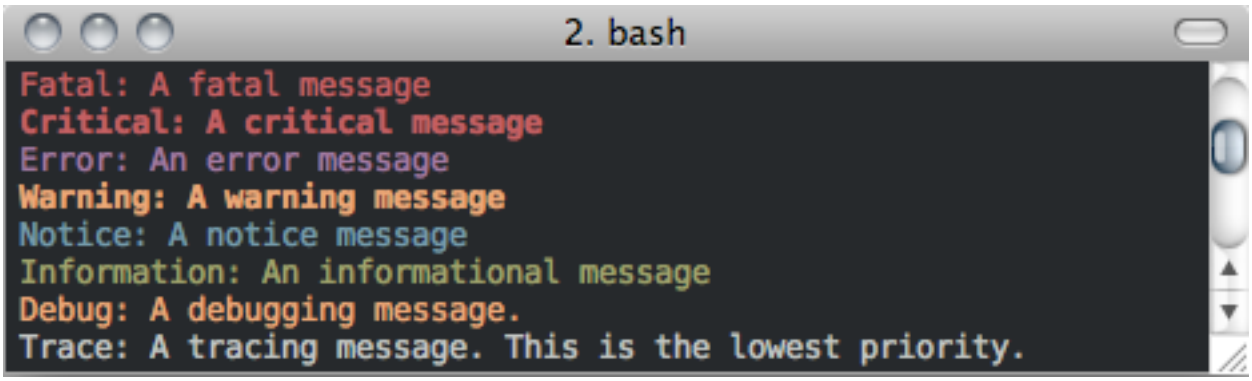
If one wants to display logging at the lowest level (LOG_TRACE), where every logging message is displayed, one would run:

```
roadrunner.Logging.setLevel(roadrunner.Logging.LOG_TRACE)
```

Logging the following messages:

```
roadrunner.Logger.log(roadrunner.Logger.LOG_FATAL, "A fatal message")
roadrunner.Logger.log(roadrunner.Logger.LOG_CRITICAL, "A critical message")
roadrunner.Logger.log(roadrunner.Logger.LOG_ERROR, "An error message")
roadrunner.Logger.log(roadrunner.Logger.LOG_WARNING, "A warning message")
roadrunner.Logger.log(roadrunner.Logger.LOG_NOTICE, "A notice message")
roadrunner.Logger.log(roadrunner.Logger.LOG_INFORMATION, "An informational message")
roadrunner.Logger.log(roadrunner.Logger.LOG_DEBUG, "A debugging message.")
roadrunner.Logger.log(roadrunner.Logger.LOG_TRACE,  "A tracing message. This is the␣
↪lowest priority.")
```

will produce the following output:



If one wants different colors on the log, these can be set via:

```
rr.Logger.setProperty("traceColor", "red")
rr.Logger.setProperty("debugColor", "green")
```

The available color property names and values are listed below at the Logger.setProperty method.

Logging Levels

The Logger has the following logging levels:

Logger.**LOG_CURRENT**
Use the current level – don't change the level from what it is.

Logger.**LOG_FATAL**
A fatal error. The application will most likely terminate. This is the highest priority.

Logger.**LOG_CRITICAL**
A critical error. The application might not be able to continue running successfully.

Logger.**LOG_ERROR**
An error. An operation did not complete successfully, but the application as a whole is not affected.

Logger.**LOG_WARNING**
A warning. An operation completed with an unexpected result.

Logger.**LOG_NOTICE**
A notice, which is an information with just a higher priority.

Logger.**LOG_INFORMATION**
An informational message, usually denoting the successful completion of an operation.

Logger.**LOG_DEBUG**
A debugging message.

Logger.**LOG_TRACE**
A tracing message. This is the lowest priority.

Logging Methods

static Logger.**setLevel**([*level*])
sets the logging level to one a value from Logger::Level

Parameters **level** (*int*) – the level to set, defaults to LOG_CURRENT if none is specified.

static Logger.**getLevel**()
get the current logging level.

static Logger.**disableLogging**()
Suppresses all logging output

static Logger.**disableConsoleLogging**()
stops logging to the console, but file logging may continue.

static Logger.**enableConsoleLogging**(*level*)
turns on console logging (stderr) at the given level.

Parameters **level** – A logging level, one of the above listed LOG_* levels.

static Logger.**enableFileLogging**(*fileName*[, *level*])
turns on file logging to the given file as the given level.

Parameters

- **fileName** (*str*) – the path of a file to log to.
- **level** – (optional) the logging level, defaults to LOG_CURRENT.

static Logger.**disableFileLogging**()
turns off file logging, but has no effect on console logging.

static Logger.**getCurrentLevelAsString**()
get the textural form of the current logging level.

static Logger.**getFileName**()
get the name of the currently used log file.

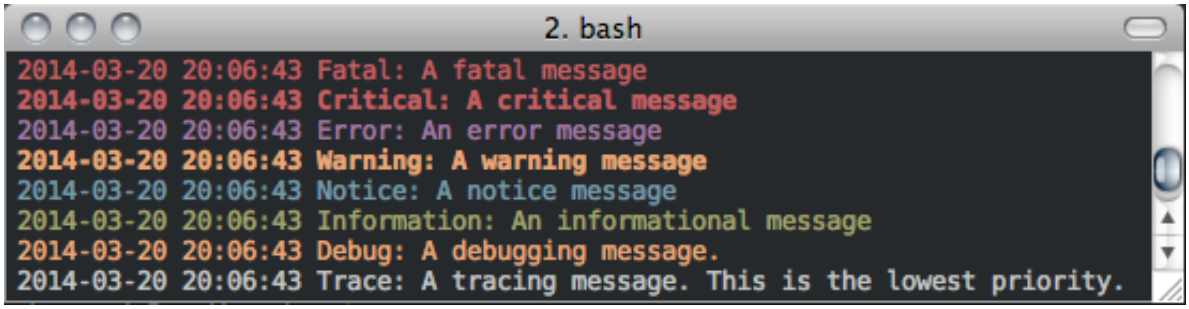
static Logger.**setFormattingPattern**(*format*)
Internally, RoadRunner uses the Poco logging framework, so we can custom format logging output based on a formatting pattern string.

The format pattern is used as a template to format the message and is copied character by character except for the following special characters, which are replaced by the corresponding value.

An example pattern of "%Y-%m-%d %H:%M:%S %p: %t" set via:

```
roadrunner.Logger.setFormattingPattern("%Y-%m-%d %H:%M:%S %p: %t")
```

would produce the following output:



RoadRunner supports the following format specifiers. These were copied from the Poco documentation:

- %s - message source
- %t - message text
- %l - message priority level (1 .. 7)
- %p - message priority (Fatal, Critical, Error, Warning, Notice, Information, Debug, Trace)
- %q - abbreviated message priority (F, C, E, W, N, I, D, T)
- %P - message process identifier
- %T - message thread name
- %I - message thread identifier (numeric)
- %N - node or host name
- %U - message source file path (empty string if not set)
- %u - message source line number (0 if not set)
- %w - message date/time abbreviated weekday (Mon, Tue, . . .)
- %W - message date/time full weekday (Monday, Tuesday, . . .)
- %b - message date/time abbreviated month (Jan, Feb, . . .)
- %B - message date/time full month (January, February, . . .)

- %d - message date/time zero-padded day of month (01 .. 31)
- %e - message date/time day of month (1 .. 31)
- %f - message date/time space-padded day of month (1 .. 31)
- %m - message date/time zero-padded month (01 .. 12)
- %n - message date/time month (1 .. 12)
- %o - message date/time space-padded month (1 .. 12)
- %y - message date/time year without century (70)
- %Y - message date/time year with century (1970)
- %H - message date/time hour (00 .. 23)
- %h - message date/time hour (00 .. 12)
- %a - message date/time am/pm
- %A - message date/time AM/PM
- %M - message date/time minute (00 .. 59)
- %S - message date/time second (00 .. 59)
- %i - message date/time millisecond (000 .. 999)
- %c - message date/time centisecond (0 .. 9)
- %F - message date/time fractional seconds/microseconds (000000 - 999999)
- %z - time zone differential in ISO 8601 format (Z or +NN.NN)
- %Z - time zone differential in RFC format (GMT or +NNNN)
- %E - epoch time (UTC, seconds since midnight, January 1, 1970)
- %[name] - the value of the message parameter with the given name
- %% - percent sign

Parameters **format** (*str*) – the logging format string. Must be formatted using the above specifiers.

static Logger.**getFormattingPattern**()
get the currently set formatting pattern.

static Logger.**levelToString**(*level*)
gets the textual form of a logging level Enum for a given value.

Parameters **level** (*int*) – One of the above listed logging levels.

static Logger.**stringToLevel**(*s*)
parses a string and returns a Logger::Level

Parameters **s** (*str*) – the string to parse.

static Logger.**getColoredOutput**()
check if we have colored logging enabled.

static Logger.**setColoredOutput**(*b*)
enable / disable colored output

Parameters **b** (*boolean*) – turn colored logging on or off

static Logger.**setProperty**(*name*, *value*)
Set the color of the output logging messages.

In the future, we may add additional properties here.

The following properties are supported:

- enableColors: Enable or disable colors.
- traceColor: Specify color for trace messages.
- debugColor: Specify color for debug messages.
- informationColor: Specify color for information messages.
- noticeColor: Specify color for notice messages.
- warningColor: Specify color for warning messages.
- errorColor: Specify color for error messages.
- criticalColor: Specify color for critical messages.
- fatalColor: Specify color for fatal messages.

The following color values are supported:

- default
- black
- red
- green
- brown
- blue
- magenta
- cyan
- gray
- darkgray
- lightRed
- lightGreen
- yellow
- lightBlue
- lightMagenta
- lightCyan
- white

Parameters

- **name** (*str*) – the name of the value to set.
- **value** (*str*) – the value to set.

static Logger.**log**(*level*, *msg*)
logs a message to the log.

Parameters

- **level** (*int*) – the level to log at.
- **msg** (*str*) – the message to log.

1.13.10 JIT Compilation

class RoadRunner.**Compiler**
The Compiler object provides information about the JIT compiler currently in use.

Compiler.**getCompiler**()
gets the name of the JIT compiler, i.e. "LLVM" means we are using the LLVM JIT compiler.

Return type str

Compiler.**getVersion**()
get the version of the JIT compiler.

Return type str

Compiler.**getDefaultTargetTriple**()
Return the default target triple the compiler has been configured to produce code for. A 'triple' is just a string that contains three items, it is called 'triple' as that is a LLVM historical convention.

The target triple is a string in the format of: CPU_TYPE-VENDOR-OPERATING_SYSTEM

or

CPU_TYPE-VENDOR-KERNEL-OPERATING_SYSTEM

Return type str

Compiler.**getProcessTriple**()
Return an appropriate target triple for generating code to be loaded into the current process, e.g. when using the JIT.

Return type str

Compiler.**getHostCPUName**()
getHostCPUName - Get the LLVM name for the host CPU. The particular format of the name is target dependent, and suitable for passing as -mcpu to the target which matches the host.

return - The host CPU name, or empty if the CPU could not be determined.

Return type str

Compiler.**setCompiler**(*compiler*)
A legacy method that currently does not do anything.

Compiler.**getCompilerLocation**()
A legacy method that currently does not do anything.

Compiler.**setCompilerLocation**(*loc*)
A legacy method that currently does not do anything.

Compiler.**getSupportCodeFolder**()
A legacy method that currently does not do anything.

Compiler.**setSupportCodeFolder**(*path*)
A legacy method that currently does not do anything.

1.13.11 Miscellaneous Functions

roadrunner.**getCopyrightStr**()
Returns the copyright string

roadrunner.**getVersionStr**()
Returns the version string

static roadrunner.**RoadRunner_getExtendedVersionInfo**()
getVersionStr() with infomation about dependent libs versions.

static roadrunner.**RoadRunner_getParamPromotedSBML**(**args*)
Takes an SBML document (in textual form) and changes all of the local parameters to be global parameters.

Parameters **SBML** (*str*) – the contents of an SBML document

Return type str

roadrunner.**validateSBML**(**args*)
Given a string, check whether the string is a valid SBML string. Raises exception if the string is not a valid SBML string.

Parameters **SBML** (*str*) – the contents of an SBML document

roadrunner.**listTestModels**()
Lists all the test models.

roadrunner.**loadTestModel**(*name*)
Load a test model given a name.

Parameters **name** (*str*) – name of the test model

CHAPTER 2

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