Tellurium and libRoadRunner in a Nutshell

Herbert M Sauro

University of Washington

hsauro@uw.washington.edu

Developed by Andy Somogyi and the software team at UW with input from Maciek Swat

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Tellurium

Tellurium is an integrated platform based on Python and spyder2. It runs on Mac, Windows and Linux. It includes the following libraries:

libRoadRunner: A high performance SBML simulation library.

Antimony: Allows user to write models in a more human readable form.

SBML2Matlab: Allows users s to export models in Matlab format

In addition Tellurium comes preloaded with the Python plotting library **Matplotlib** and the array package **numpy**. Tellurium also comes with a small number of helper subroutines to make it easier for the average modeler.

Download the Software

To download the software go to the web site:

`http://tellurium.analogmachine.org/`

Pick the download that is appropriate for your computer.

Do this now.....

First Example

Example

```
import tellurium as te

r = te.loada ('''
    S1 -> S2; k1*S1;
    S2 -> S3; k2*S2;

    k1 = 0.1; k2 = 0.45;
    S1 = 10; S2 = 0; S3 = 0
''')

result = r.simulate (0, 40, 100)
r.plot (result)
```

Antimony

Example (Simple Model)

```
S1 -> S2; k1*S1;

k1 = 0.1; S1 = 10; S2 = 0
```

$$\frac{dS1}{dt} = -k_1 S_1$$

$$\frac{dS2}{dt} = k_1 S_1$$

Antimony

Example (Multiple Reactions)

```
S1 -> S2; k1*S1;
S2 -> S3; k2*S2;

k1 = 0.1; k2 = 0.2;
S1 = 10; S2 = 0; S3 = 0
```

$$\frac{dS1}{dt} = -k_1 S_1$$

$$\frac{dS2}{dt} = k_1 S_1 - k_2 S_2$$

$$\frac{dS3}{dt} = k_2 S_2$$

Antimony

Example (Rate Laws)

```
S1 -> S2; k1*S1 - k2*S2;      # Reversible
S2 -> S3; Vmax*S3/(Km + S3); # Michaelis-Menten

k1 = 0.1; k2 = 0.2; Vmax = 10; Km = 0,4
S1 = 10; S2 = 0; S3 = 0
```

Antimony

Example (Bimolecular Reactions)

```
S1 + S2 -> S3; k1*S1*S2;
S3 -> S4 + S4; k2*S3;

k1 = 0.1; k2 = 0.2;
S1 = 10; S2 = 0; S3 = 0
```

Antimony

Example (Fixed Species)

```
# This is a comment
# A $ means FIX the concentration of the species
$S1 -> S2; k1*S1;
S2 -> $S3; k2*S2;

k1 = 0.1; k2 = 0.2;
S1 = 10; S2 = 0; S3 = 0
```

Example (Events)

```
# This is a comment
# A $ means FIX the concentration of the species
$S1 -> S2; k1*S1;
S2 -> $S3; k2*S2;

at (time > 5): k2 = k2*2;

k1 = 0.1; k2 = 0.2;
S1 = 10; S2 = 0; S3 = 0
```

Antimony

Example (Named Reactions)

```
# Name reactions are useful for getting the reaction rates
J1: $S1 -> S2; k1*S1;
J2: S2 -> $S3; k2*S2;

k1 = 0.1; k2 = 0.2;
S1 = 10; S2 = 0; S3 = 0
```

Antimony

Example (Loading a Model into libRoadRunner)

```
import tellurium as te
r = te.loada ('''
  J1: $S1 -> S2; k1*S1;
  J2: S2 -> $S3; k2*S2;

  k1 = 0.1; k2 = 0.2;
  S1 = 10; S2 = 0; S3 = 0
''')
```

Antimony

Example (Standard import boiler plate)

```
import tellurium as te
import numpy
import roadrunner
import matplotlib.pyplot as plt
```

Antimony

Example (Run a Simulation)

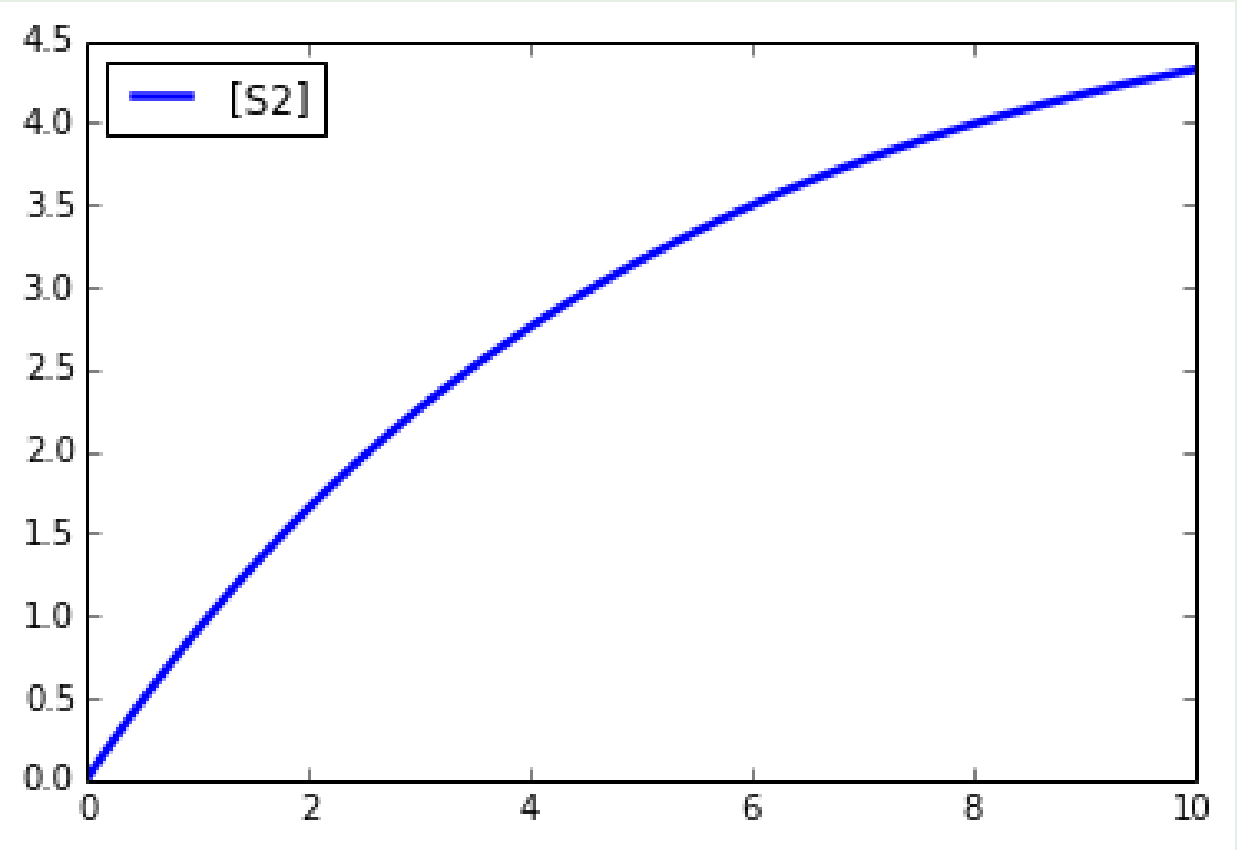
```
r = te.loada ('''
  J1: $S1 -> S2; k1*S1;
  J2: S2 -> $S3; k2*S2;

  k1 = 0.1; k2 = 0.2;
  S1 = 10; S2 = 0; S3 = 0
''')

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

Antimony

Example (Plotting Results)

```
r = te.loada ('''
  J1: $S1 -> S2; k1*S1;
  J2: S2 -> $S3; k2*S2;

  k1 = 0.1; k2 = 0.2;
  S1 = 10; S2 = 0; S3 = 0
''')

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

Example (Plotting Results)



Antimony

Example (Changing Values)

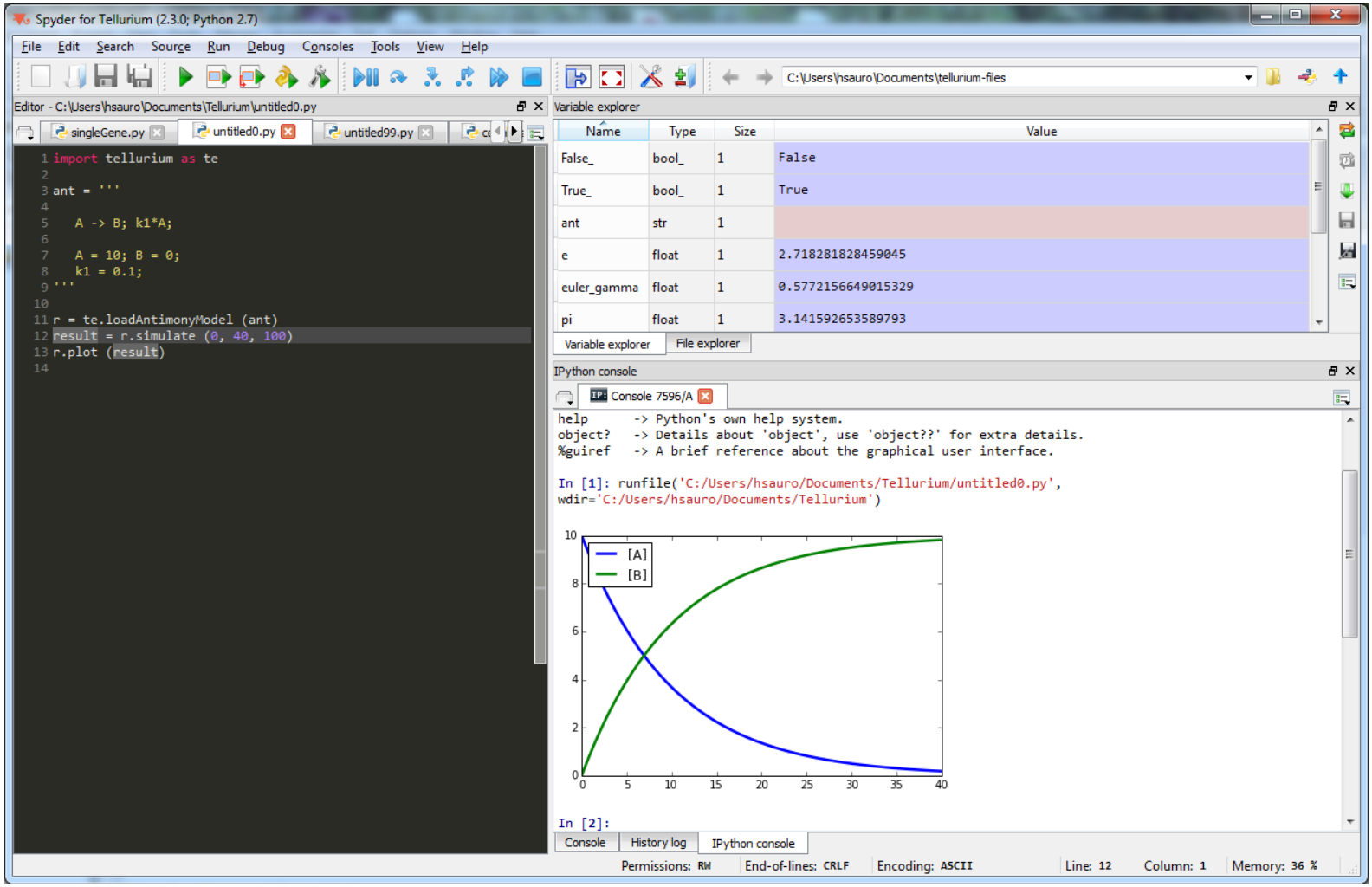
```
r = te.loada ('''
  J1: $S1 -> S2; k1*S1;
  J2: S2 -> $S3; k2*S2;

  k1 = 0.1; k2 = 0.2;
  S1 = 10; S2 = 0; S3 = 0
''')

r.model.k1 = 12.3
r.model.S1 = 20
result = r.simulate (0, 10, 100)
r.plot (result)
```

Example (Resetting the Model)

```
r = te.loada ('''
  J1: $S1 -> S2; k1*S1;
  J2: S2 -> $S3; k2*S2;

  k1 = 0.1; k2 = 0.2;
  S1 = 10; S2 = 0; S3 = 0
''')

result = r.simulate (0, 10, 100)

r.reset()  # Reset to species initial conditions
r.resetAll() # Reset initial conditions and parameter values
r.resetToOrigin() # Reset back to when the model was loaded
```

Demo

Telluirum.RoadRunner Interface



Documentation

Go to:

tellurium.analogmachine.org

and

libroadrunner.org

Exercise

Build a model that describes two consecutive reactions, each reaction governed by the simple Michaelis-Menten rate law

$$v = V_m \frac{S}{K_m + S}$$

$$\$S_1 \rightarrow S_2 \rightarrow \$S_3$$

Note S_1 and S_3 are FIXED. Set the parameters and species to:

```
Km1 = 0.5; Km2 = 0.5;
S1 = 10; S2 = 0; S3 = 0;
Vm1 = 30; Vm2 = 20;
```

Load the model into libroadrunner and run a simulation from time zero to time 10 time units. Plot the results. Explain what you observe. Set Vm1 = 18 and rerun the simulation, explain the results.

SBML

The Systems Biology Markup Language (SBML) is a representation format, based on XML, for communicating and storing computational models of biological processes. It is a free and open standard with widespread software support. SBML can represent many different classes of biological phenomena, including metabolic networks, cell signaling pathways, regulatory networks, infectious diseases, and many others. As an XML format, SBML is not meant to be read or written by Humans.