

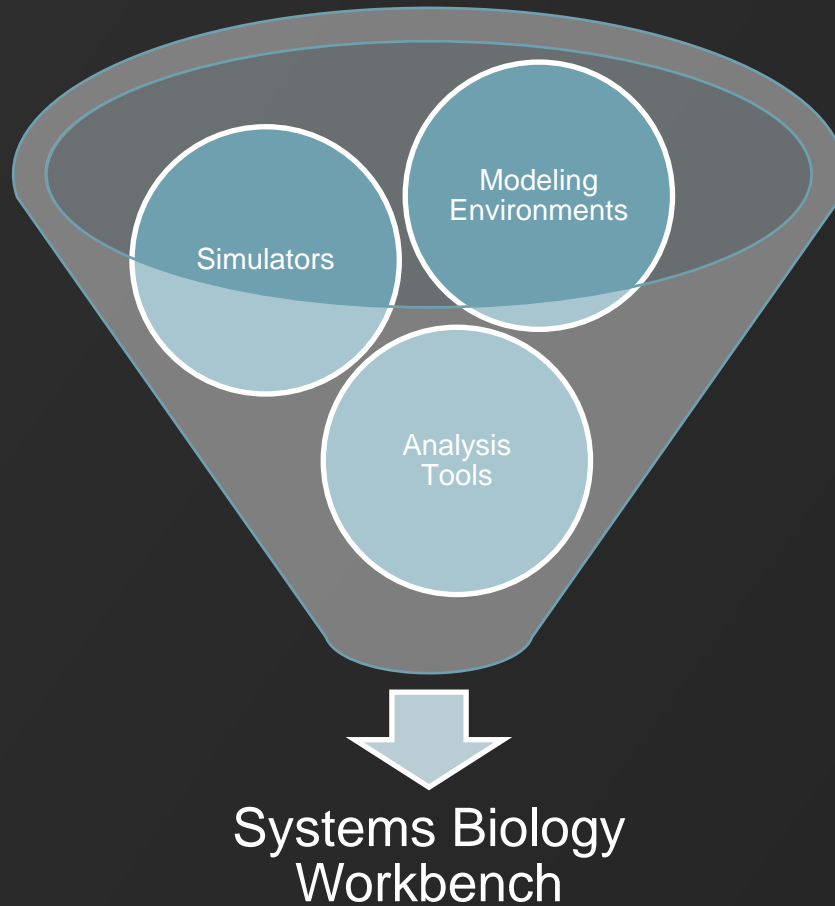
KECK GRADUATE INSTITUTE
of Applied Life Sciences



Frank Bergmann

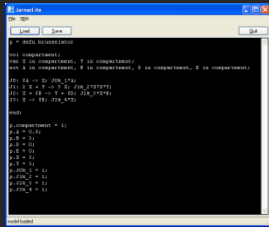
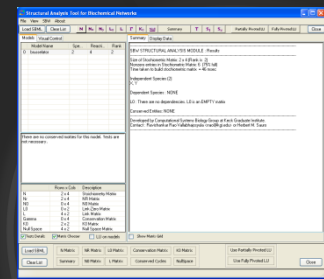
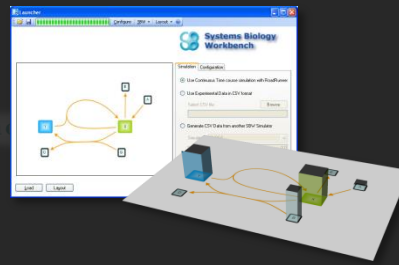
UPDATES – SYSTEMS BIOLOGY WORKBENCH

Systems Biology Workbench



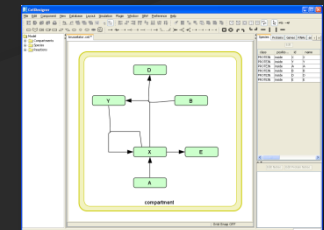
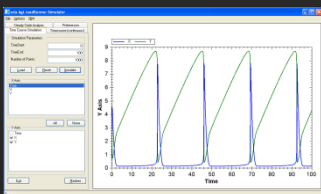
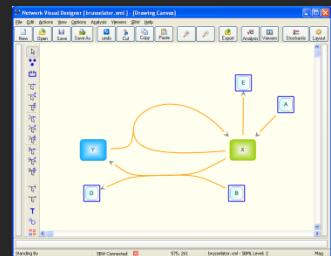
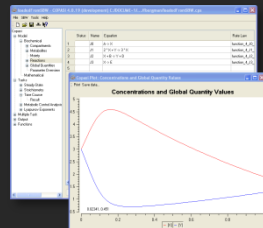
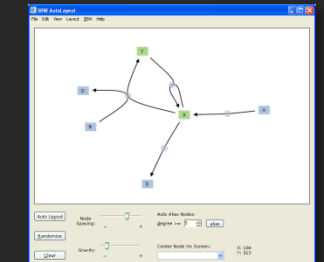
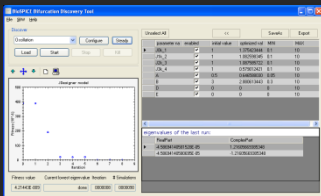
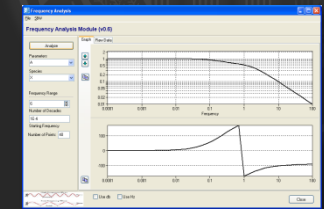
Systems Biology
Workbench

SBW Menu



SBW

- Bifurcation Discovery Tool
- Chemical_Langevin_Equation Simulation Service
- COPASI (SBW Dev. Version)
- CVODE Simulation Service
- Dizzy Simulation Service
- edu.kgi.roadRunner Simulation Service
- Frequency Analysis Module
- Gibson_NRM Simulation Service
- Gillespie_DM Simulation Service
- Gillespie_FRM Simulation Service
- GillespieGUI
- JacobianViewer
- Jarnac Simulation Service
- JDesigner
- Layout Network
- LSODA Simulation Service
- Oscill8 GUI
- Save Model as Matlab ODE Function File
- Save Model as Matlab Simulink Function File
- SBML layout reader (GUI)
- Simulate 3D (OpenGL)
- Structural Analysis Tool



Funding



DOE GENOMICS:GTL

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DISCOVERY FOR ENERGY
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U.S. DEPARTMENT OF ENERGY





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Web Applications

- Simulation
- Validation
- Layout Generation

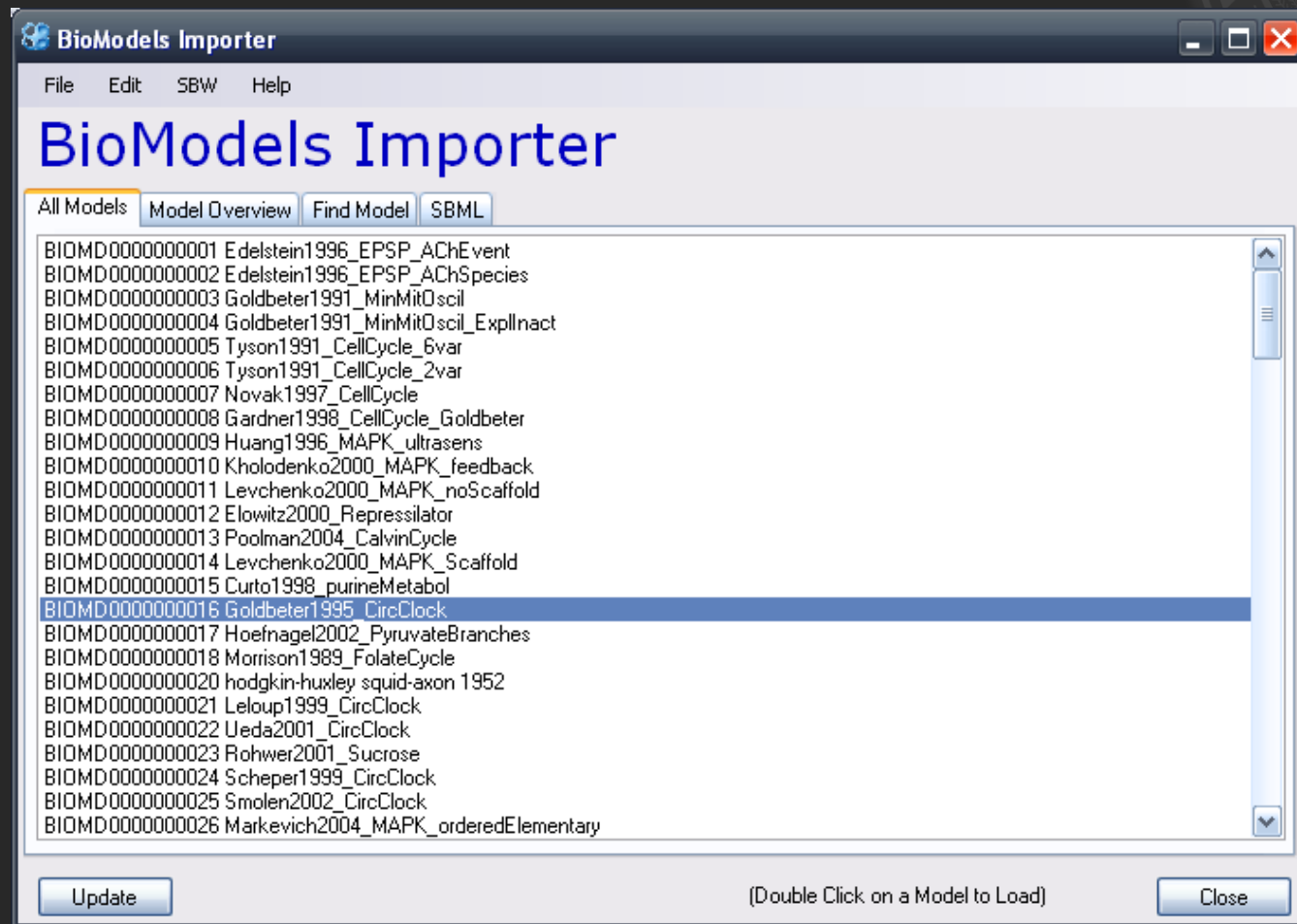
Video Tutorials

- Jarnac
- JDesigner

Updated Documentation



New Modules



New Modules

The screenshot shows the BioModels Importer application window. The title bar reads "BioModels Importer". The menu bar includes "File", "Edit", "SBW", and "Help". The main title is "BioModels Importer". Below the title, there are tabs for "All Models", "Model Overview", "Find Model", and "SBML". The "Model Overview" tab is active, showing the following details:

Id: repressilator
Name: Elowitz2000_Repressilator

Model Overview

# Floating Species	6
# Boundary Species	0
# Compartments	1
# Rules	0
# User Defined Functions	0
# Reactions	12
# Events	0

Buttons: Edit (visually), Edit (script), Simulate, Translate

Repressilator: A synthetic oscillatory network of transcriptional regulators

Citation
Elowitz MB, Leibler S (2000)
A synthetic oscillatory network of transcriptional regulators.
Nature.403 : 335 - 338.
[http:// www.nature.com/cgi-taf/DynaPage.taf?file=/nature/journal/v403/n6767/full/ 403335a0_fs.html](http://www.nature.com/cgi-taf/DynaPage.taf?file=/nature/journal/v403/n6767/full/403335a0_fs.html)

Description
This file describes the repressilator system.

The authors of this model (see reference) use three transcriptional

Buttons: Update, (Double Click on a Model to Load), Close



New Modules

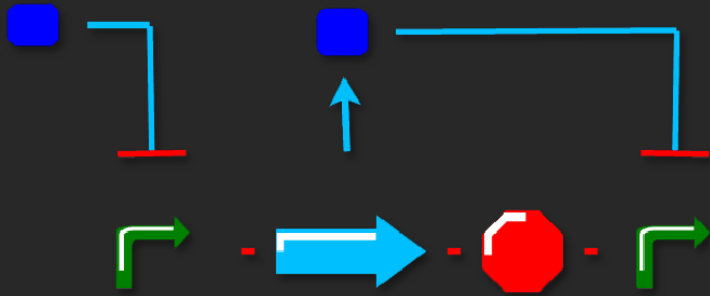
The screenshot displays the BioModels Importer application window. The main window title is "BioModels Importer" and it has a menu bar with "File", "Edit", "SBW", and "Help". Below the menu bar, the text "BioModels Importer" is prominently displayed. There are four tabs: "All Models", "Model Overview", "Find Model", and "SBML", with "SBML" currently selected. The main content area shows an SBML model snippet with the following structure:

```
-<sbml metaid="_153818"level="2"version="1">
-<model metaid="_000001" id="repressilator" name="Elowitz2000_Repressilator">
+<notes>
+<annotation>
+<listOfUnitDefinitions>
+<listOfCompartments>
-<listOfSpecies>
+<species metaid="PX" id="PX" name="Lactose operon
repressor" compartment="cell" initialAmount="5" hasOnlySubstanceUnits="true">
+<species metaid="PY" id="PY" name="Tetracycline
repressor" compartment="cell" initialAmount="0" hasOnlySubstanceUnits="true">
+<species metaid="PZ" id="PZ" name="Repressor protein
CI" compartment="cell" initialAmount="15" hasOnlySubstanceUnits="true">
-<species metaid="_905769" id="X" name="transcript
LacI" compartment="cell" initialAmount="0" hasOnlySubstanceUnits="true">
-<annotation>
-<rdf:RDF>
-<rdf:Description rdf:about="#_905769">
```

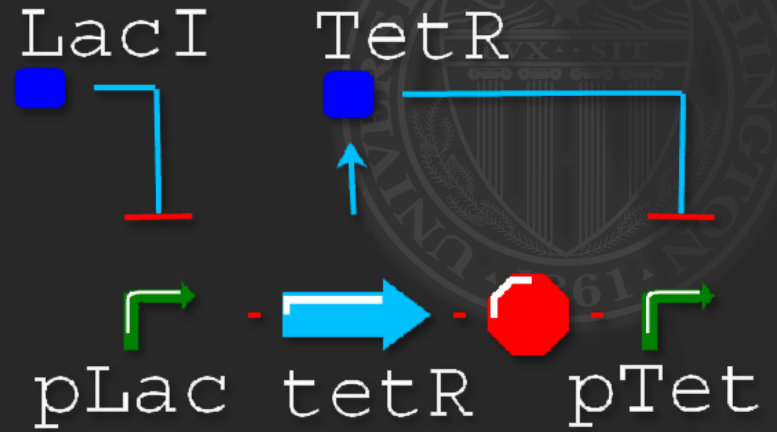
A "Find" dialog box is open over the main window, with the search term "cell" entered in the "Find:" field. Below the search field are two checkboxes: "Match whole word only" and "Match case", both of which are currently unchecked. At the bottom of the dialog box are two buttons: "Previous" and "Next".

At the bottom of the BioModels Importer window, there is an "Update" button on the left, a status message "(Double Click on a Model to Load)" in the center, and a "Close" button on the right.

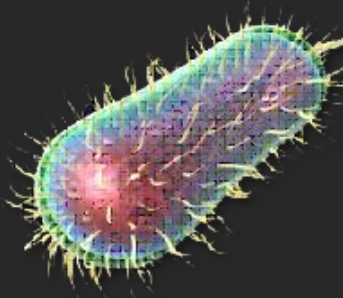
Visual Editor



Plan



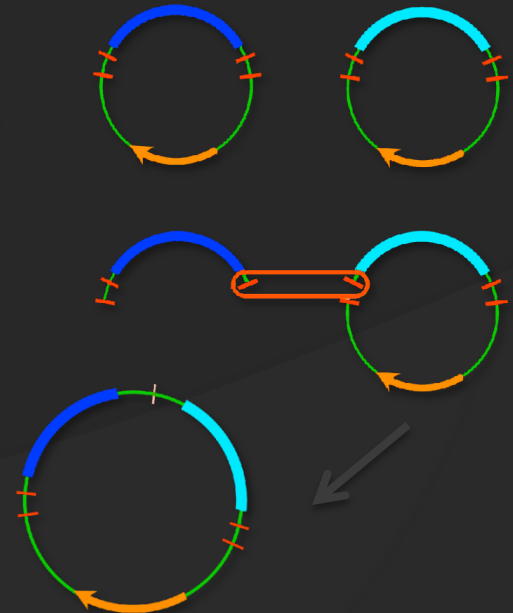
Design



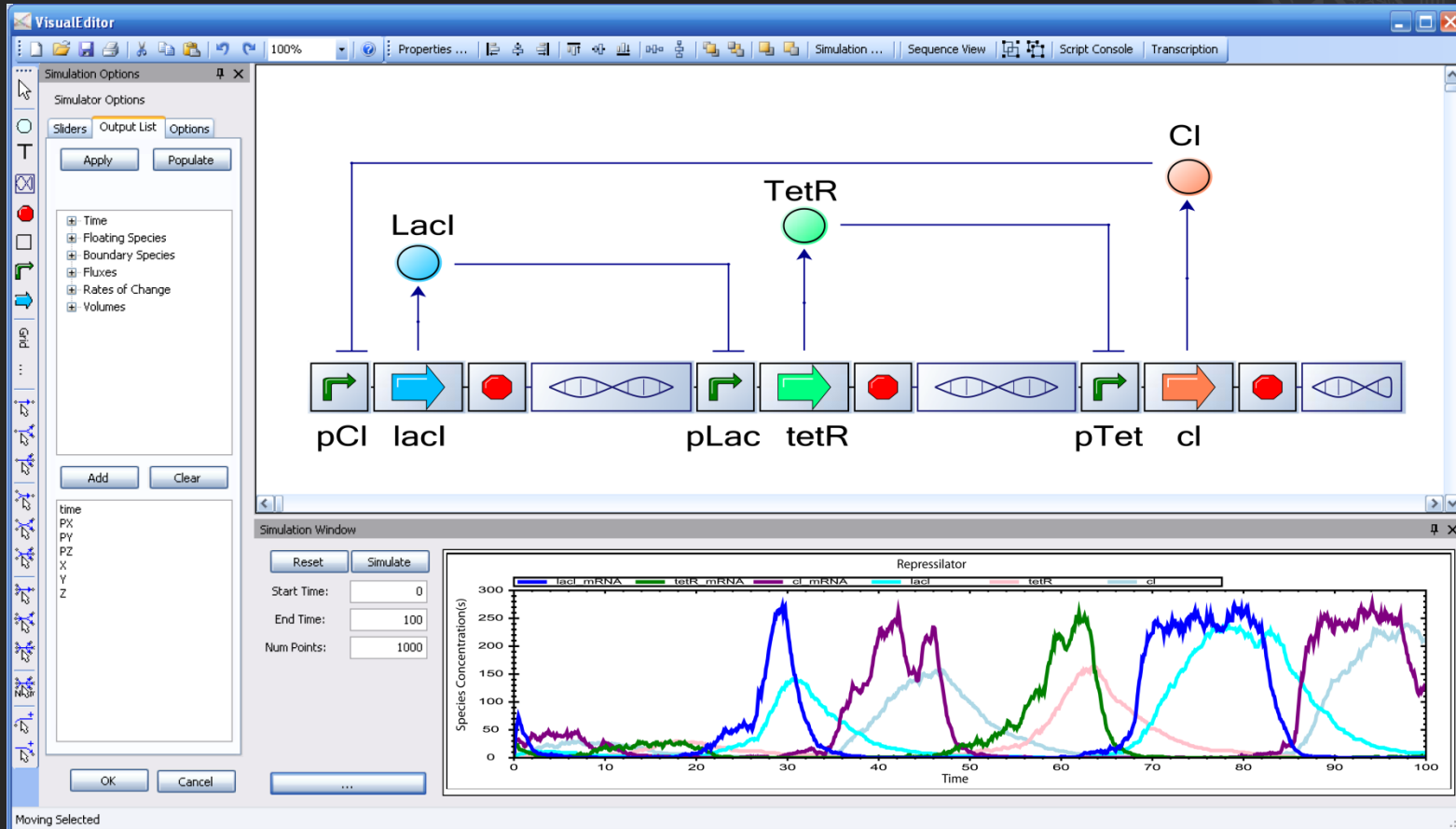
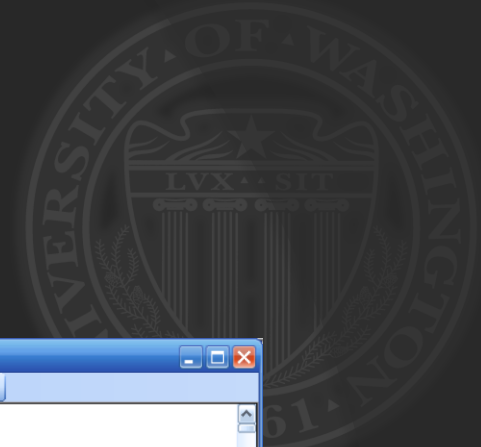
3D SCIENCE.COM

Implement

Construct



Visual Editor



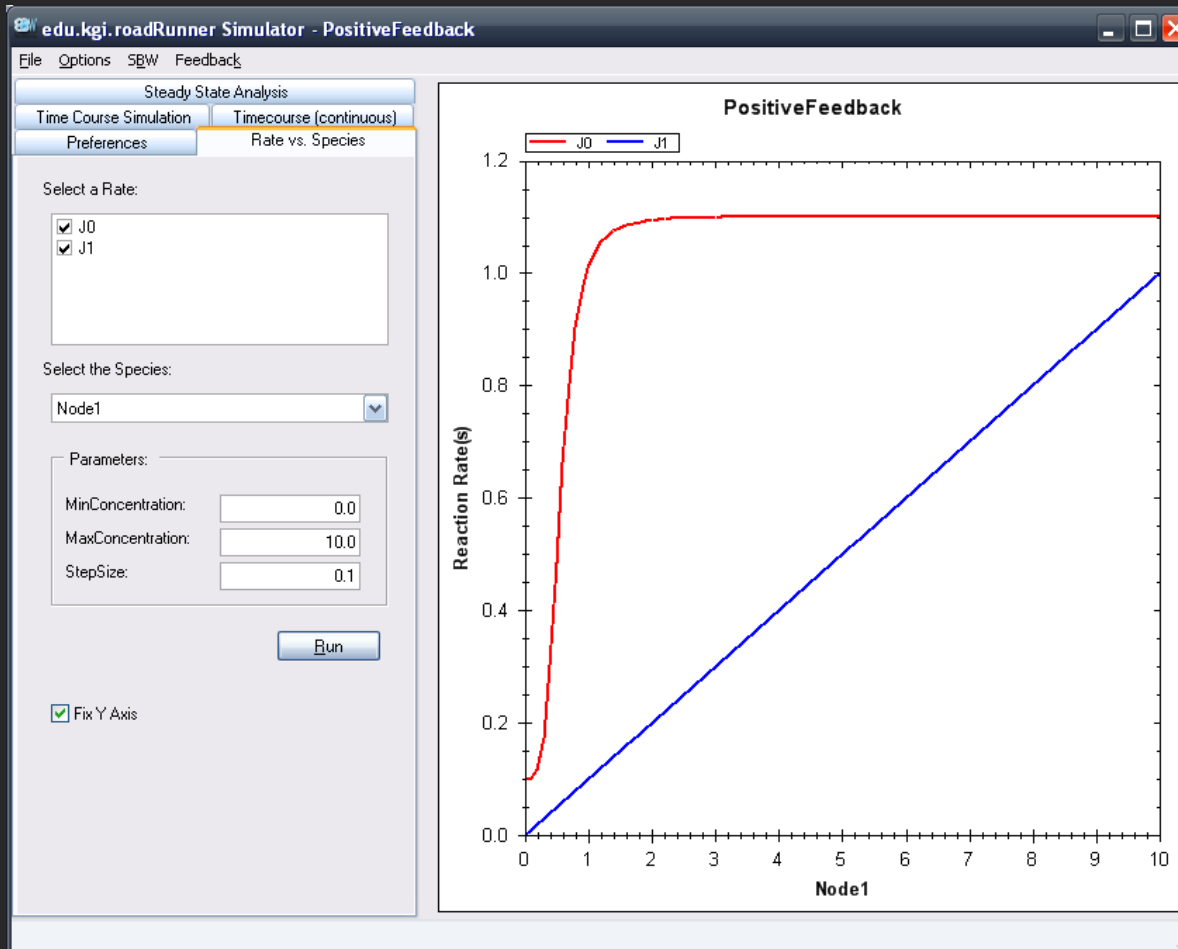
Updated Modules



SBML Support

- Using libSBML 3.0

Updated Modules



Sliders

To change one of the parameters below, click on the parameter. A slider and a textbox will appear, moving the slider, or entering a value, will instantaneously change the value in the Simulator.

Available Parameters:

- Boundary Species
- Parameters
 - J0_k: 0.1
 - k3: 4** k3
 - k2: 0.1
 - k4: 0.1
 - J1_k: 0.1

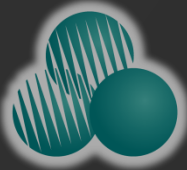
Reset Close

Updated Modules

The image displays the roadRunner Simulator interface for a 'PositiveFeedback' model. The main window is titled 'edu.kgi.roadRunner Simulator - PositiveFeedback' and contains a control panel on the left and a graph on the right. The control panel includes tabs for 'Steady State Analysis', 'Time Course Simulation', and 'Timecourse (continuous)'. Under 'Timecourse (continuous)', there are sub-tabs for 'Preferences' and 'Rate vs. Species'. The 'Rate vs. Species' tab is active, showing a 'Select a Rate:' section with checkboxes for J0 and J1, and a 'Select the Species:' dropdown menu set to 'Node1'. Below this are 'Parameters:' for 'MinConcentration' (0.0), 'MaxConcentration' (10.0), and 'StepSize' (0.1). A 'Run' button and a 'Fix Y Axis' checkbox are also present.

The graph, titled 'PositiveFeedback', plots 'Reaction Rate(s)' on the y-axis (0.0 to 1.2) against 'Node1' on the x-axis (0 to 10). Two curves are shown: a red curve for J0 and a blue curve for J1. The red curve (J0) rises sharply from 0 at x=0, reaches a plateau of approximately 0.85 at x=1, and remains constant thereafter. The blue curve (J1) rises linearly from 0 at x=0, reaching a value of 1.2 at x=4.

To the right of the main window is a 'Sliders' panel. It contains a list of 'Available Parameters' under 'Boundary Species' and 'Parameters'. The 'Parameters' section lists: J0_k: 0.0816, k3: 8.868, k2: 0.1, k4: 0.0294, and J1_k: 0.3. The J1_k parameter is highlighted with a blue box, and its value is shown in a text box as 0.3. Below the text box is a slider control with a green arrow pointing to the right, and numerical input fields for 0 and 0.3. At the bottom of the sliders panel are 'Reset' and 'Close' buttons.



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Thank You!

<http://sys-bio.org>