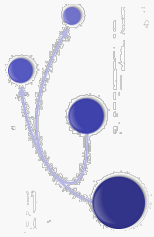
Herbert Sauro

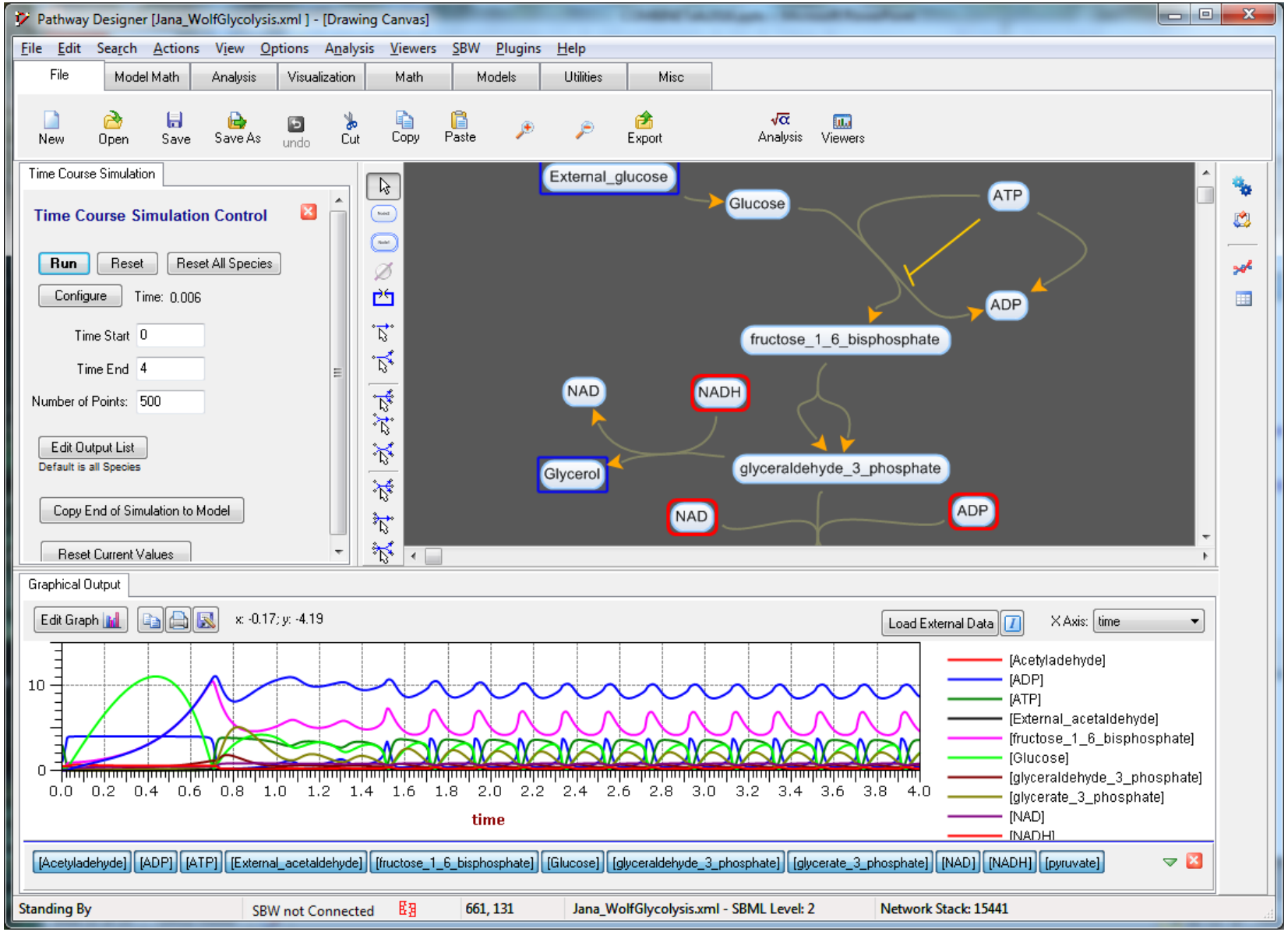
pathwayDesigner.org

Bioengineering, UW
Seattle
2016



Bosley LLC and Rosa and Co, LLC

pathwayDesigner



pathwayDesigner

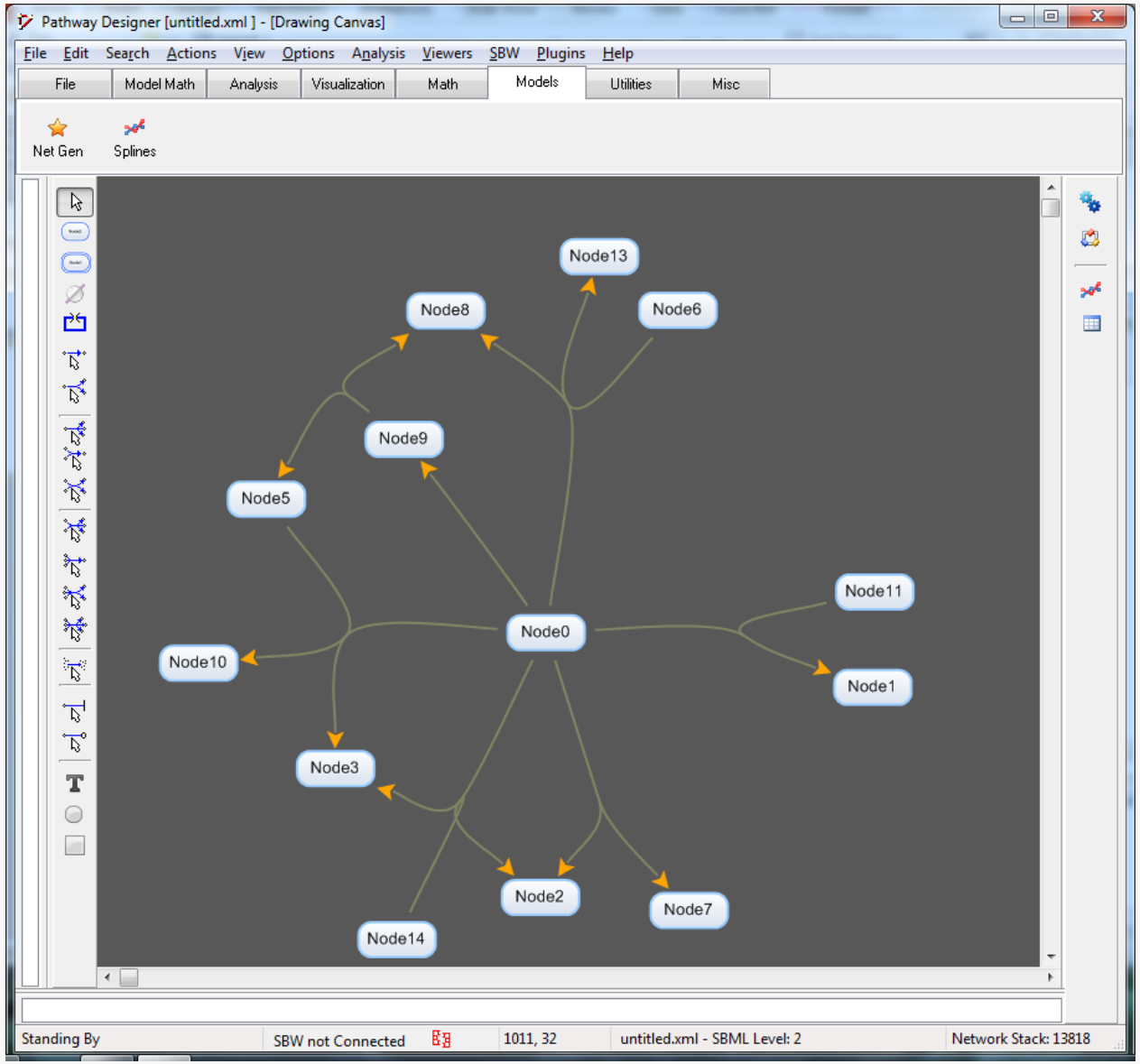
Derived from the JDesigner Codebase

Visible

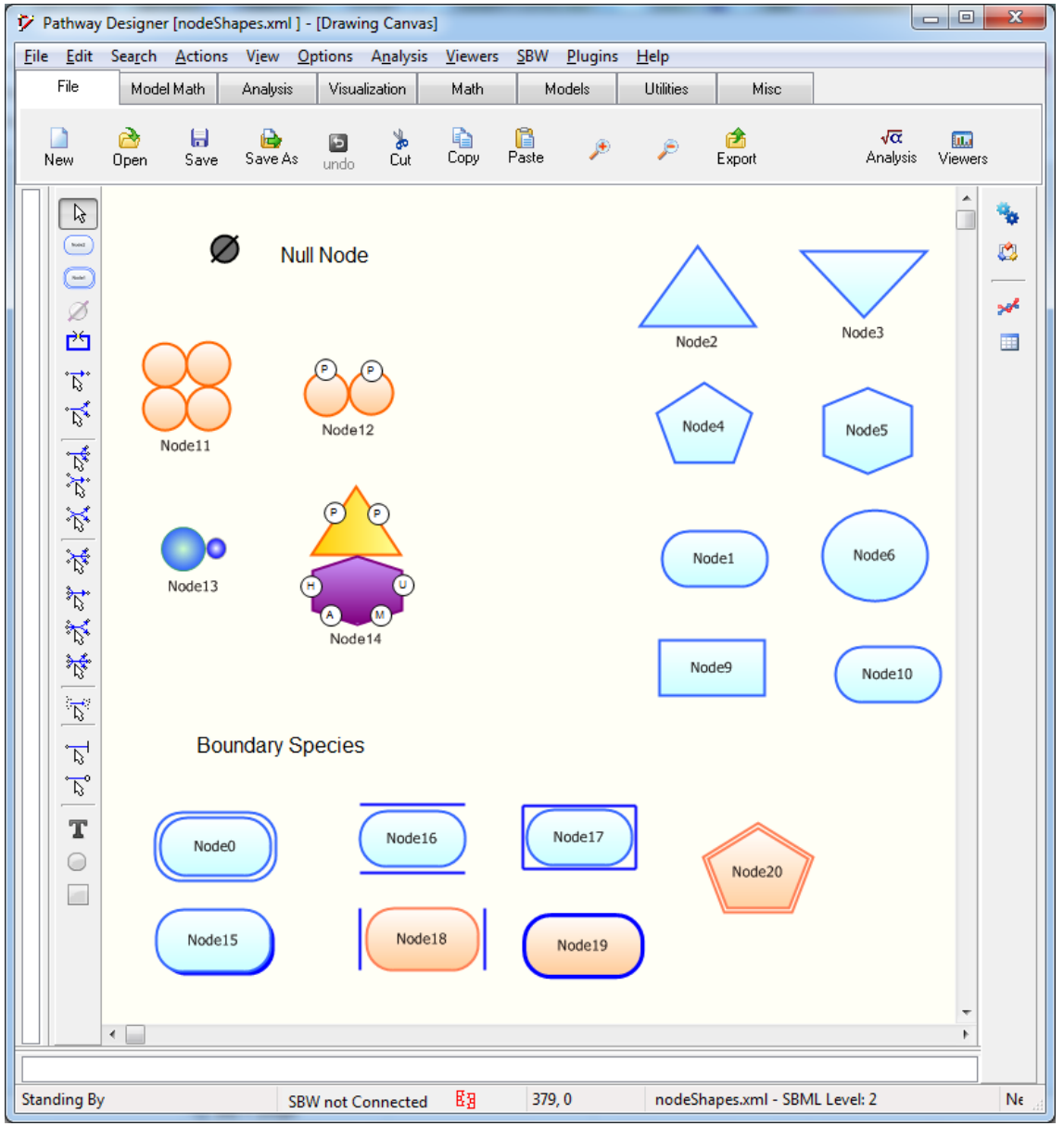
New toolbar
Range of Plugins
New range of species shapes
Styles
SBML Events
Misc

Under the Hood

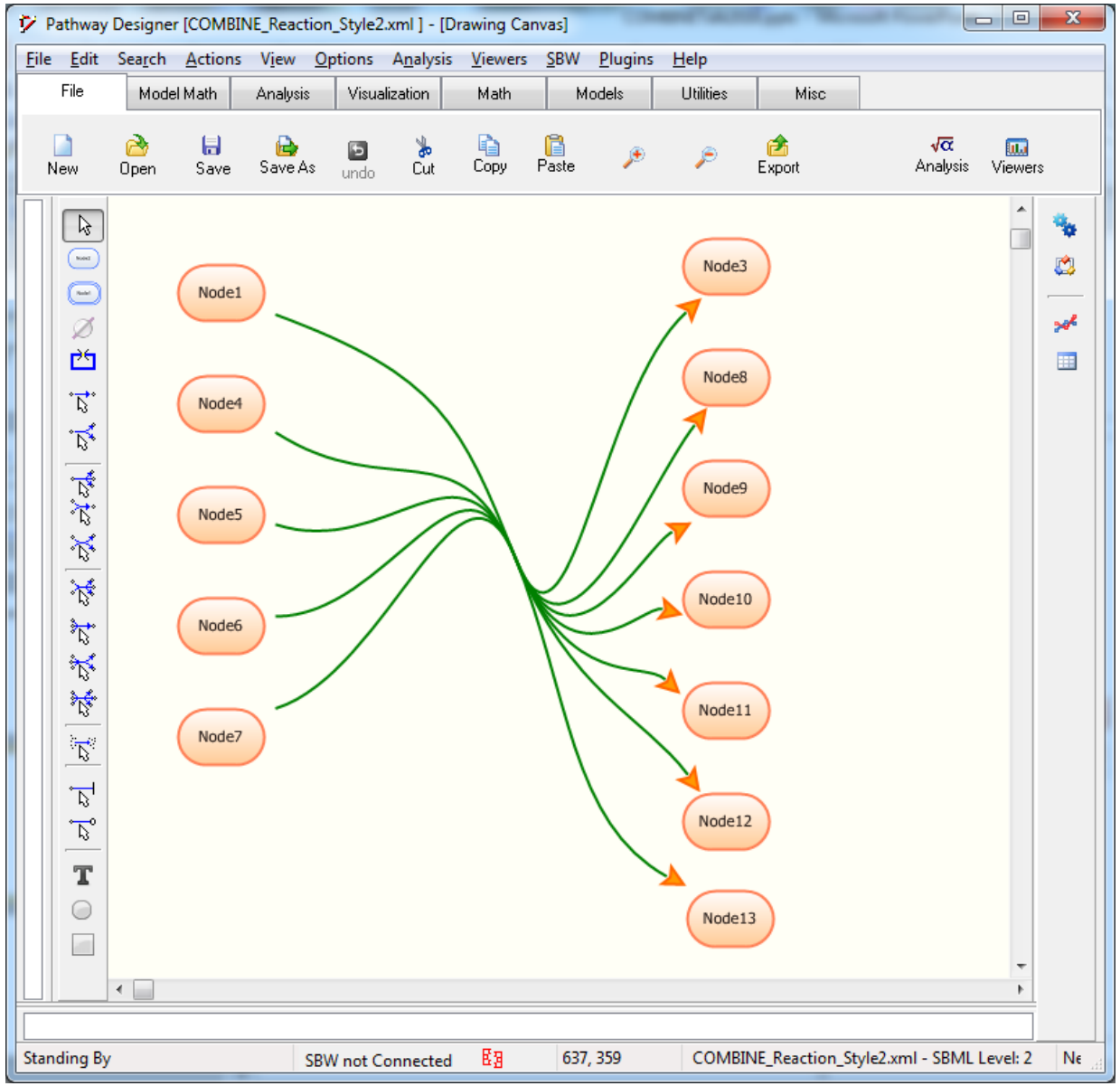
New Plugin Interface
Uses libSBML to parse SBML
Uses libRoadRunner directly
SBW interface

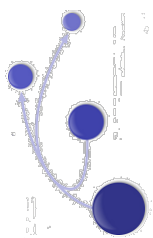


New Node Styles

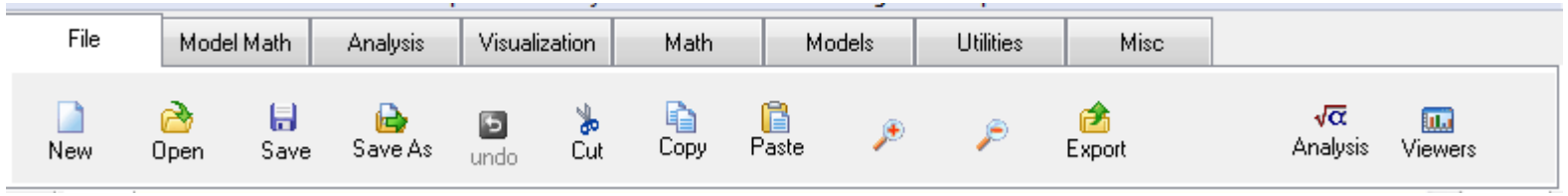


n by m reactions



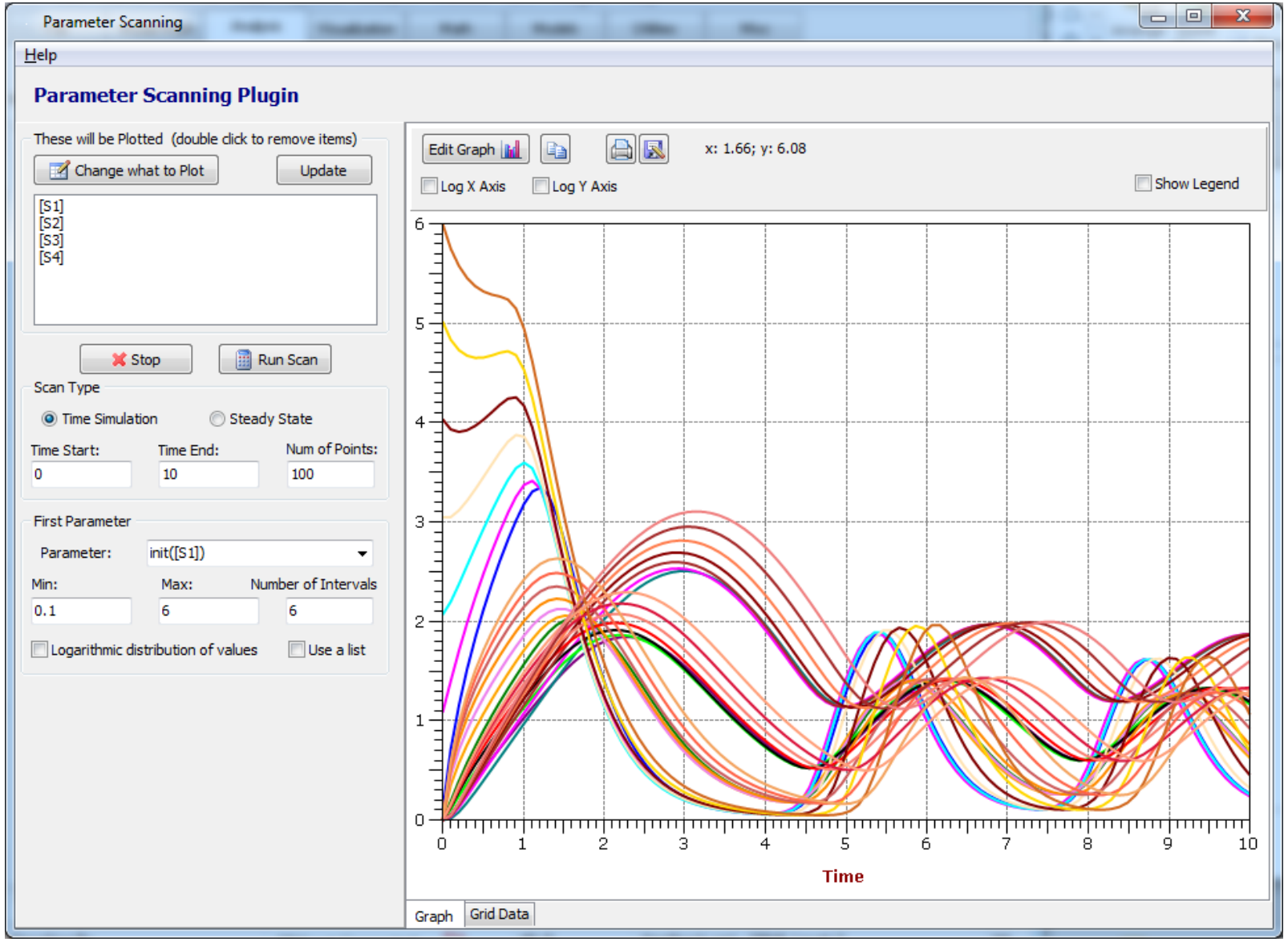


Toolbar

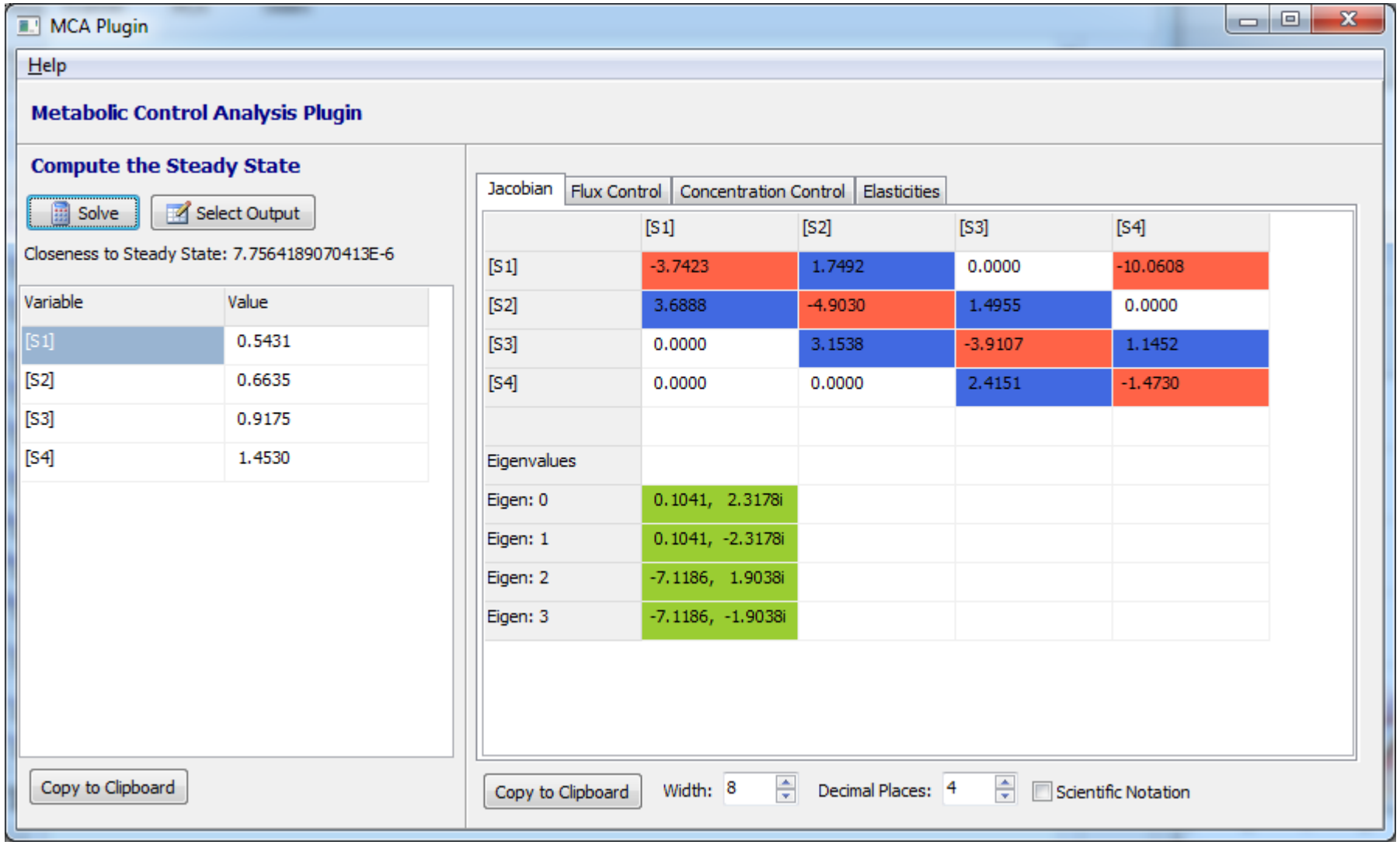


Place holder for plugins

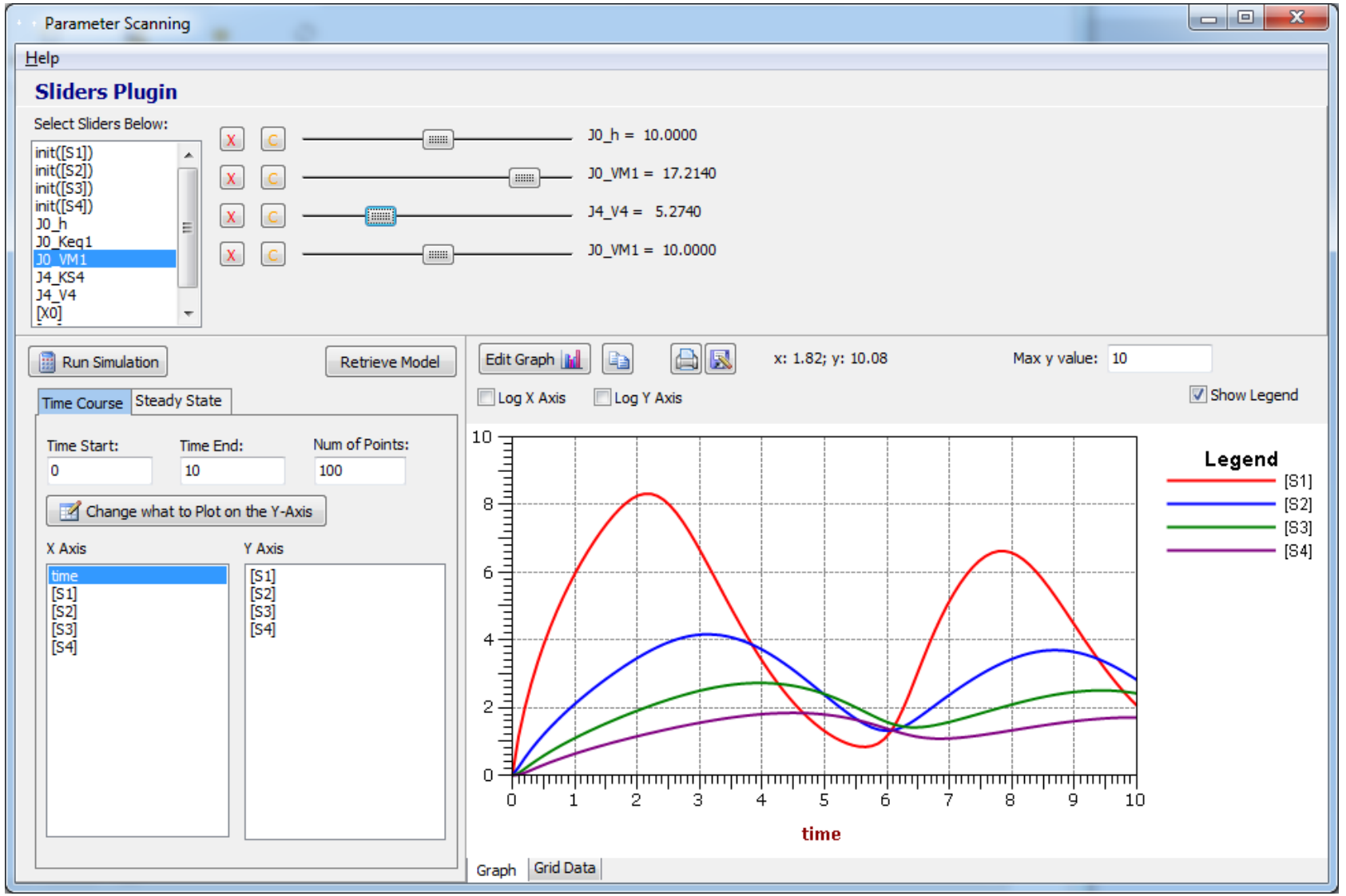
Plugins: Parameter Scanning



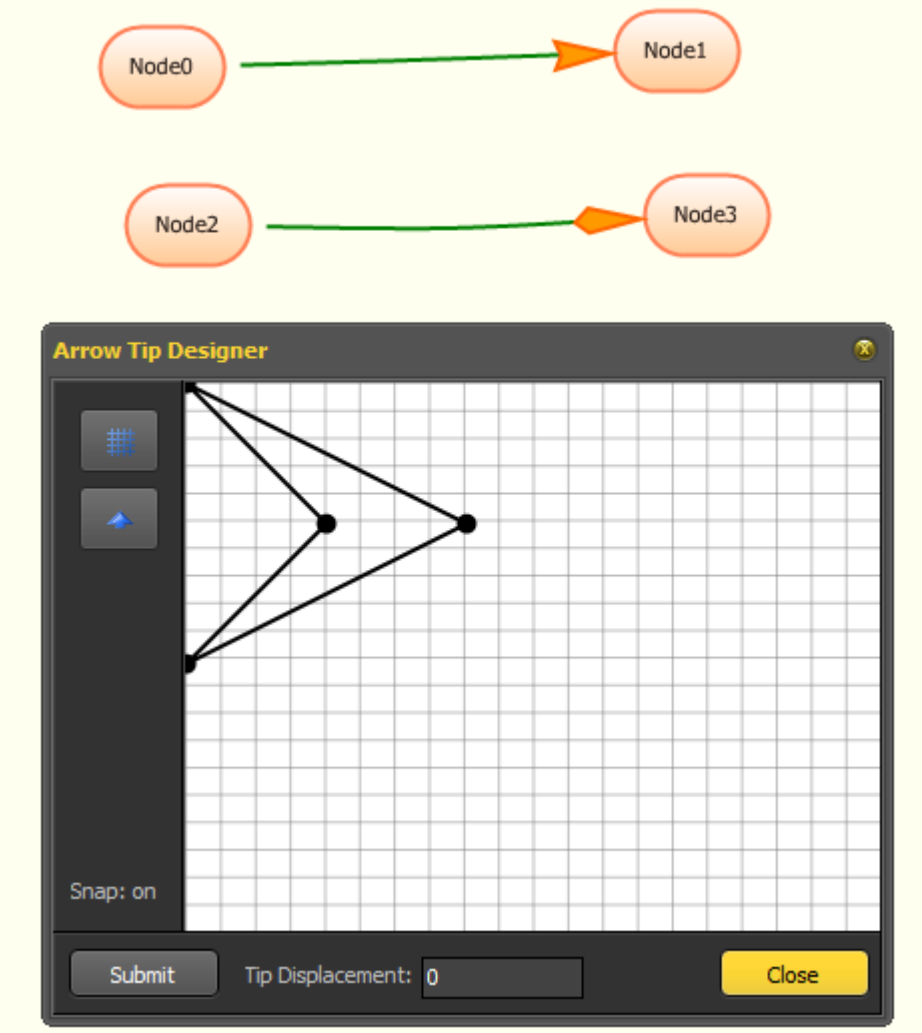
Plugins: MCA (sensitivity) Plugin



Plugins: Sliders



Plugins: Arrow Designer



AutoLayout Library

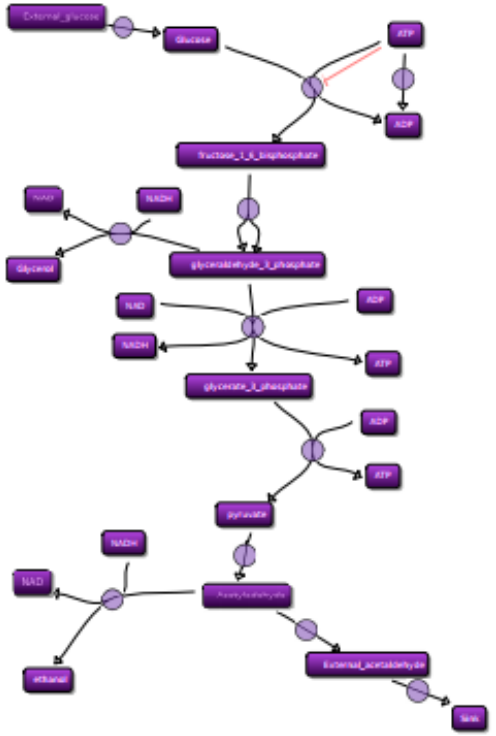
libSBNW, a portable C/C++ library that supports the SBML **layout extension** and can automatically generate layouts for SBML models. Supports layout of species, reactions, compartments and modifiers. Also includes support for alias nodes and locking of nodes in place. Python bindings are available, see Tellurium.

A portable library to support the SBML Layout Extension

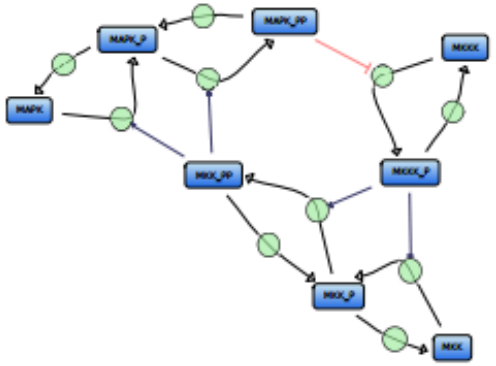
http://biorxiv.org/content/early/2016/01/05/035725

https://github.com/sys-bio/sbnw

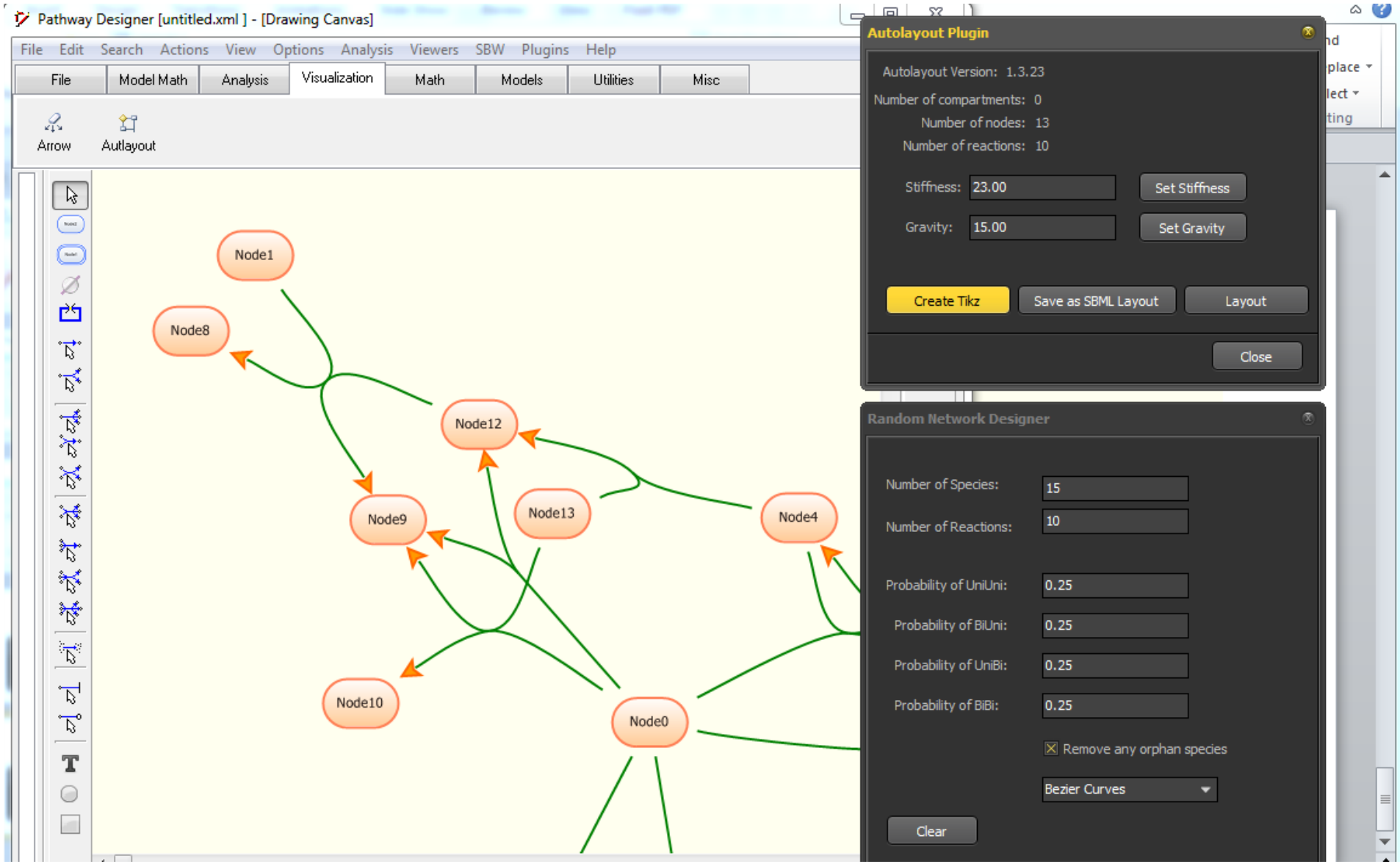
Kyle Medley



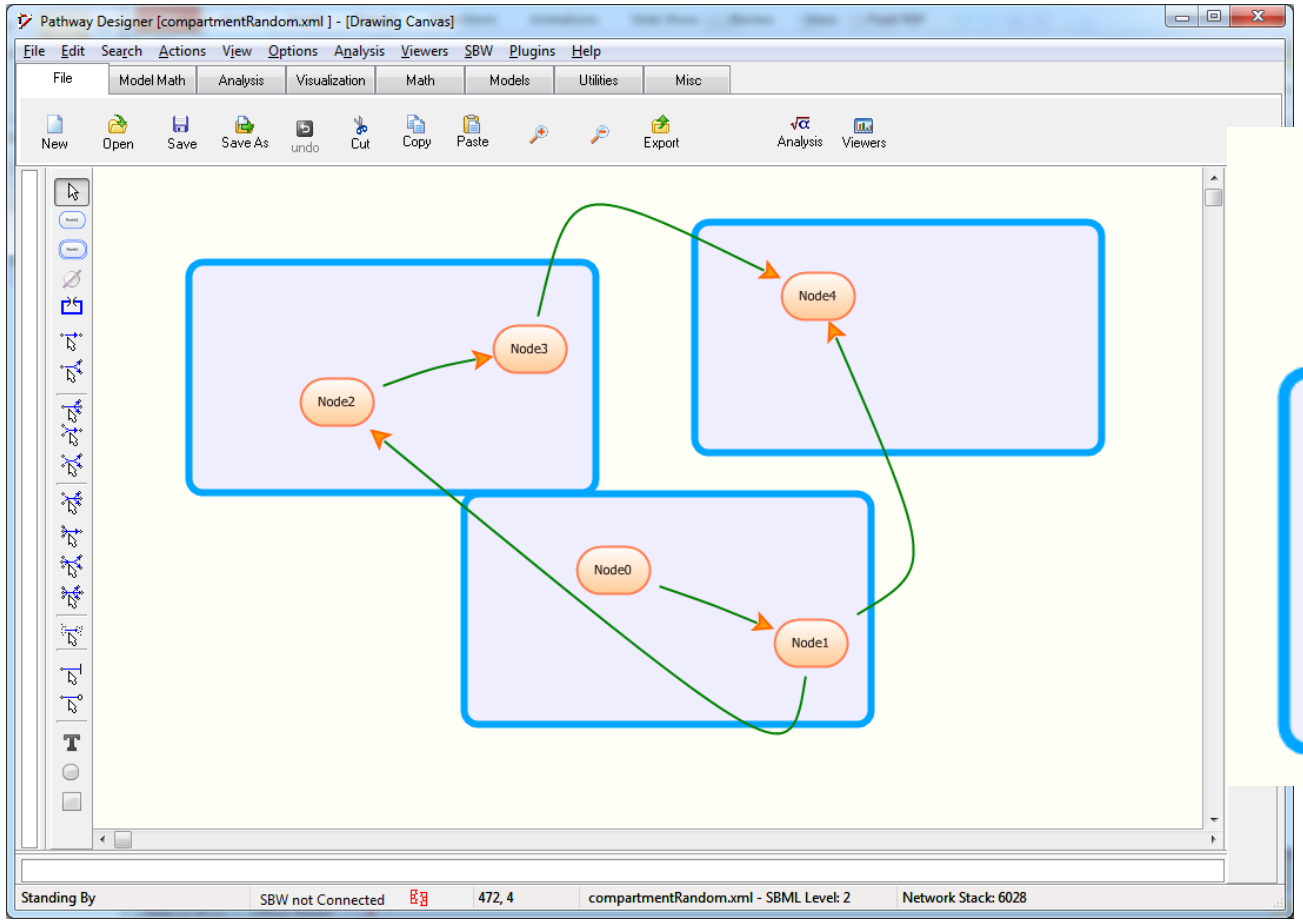
(b) A rendered version of the model displayed above

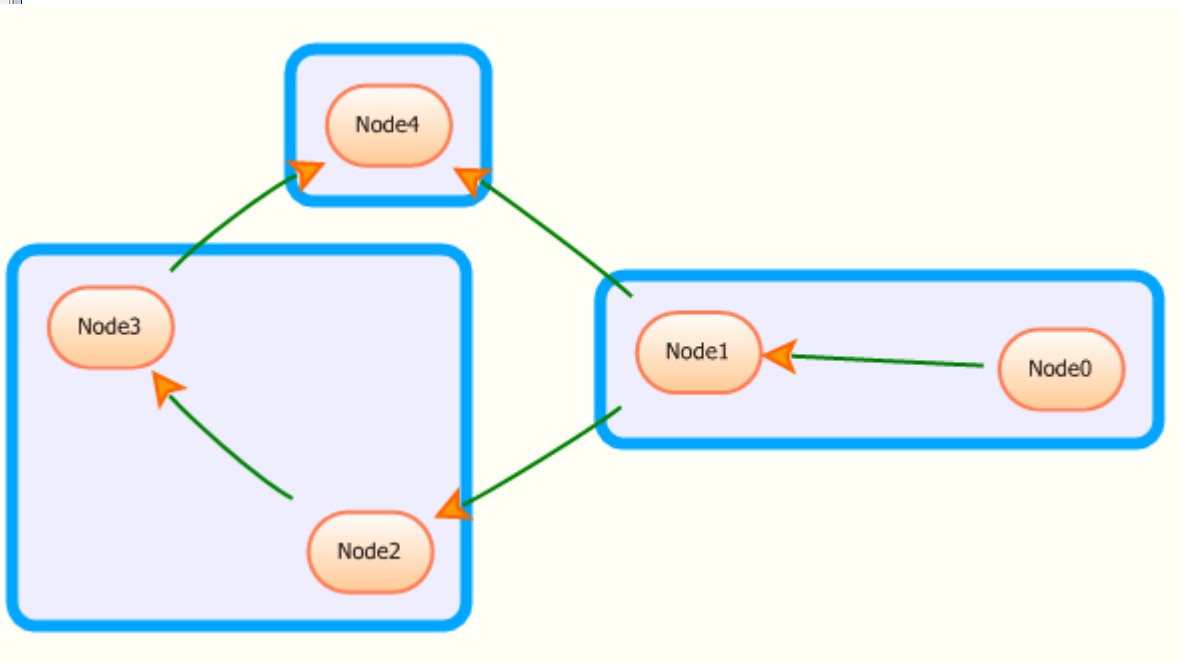


Plugins: AutoLayout

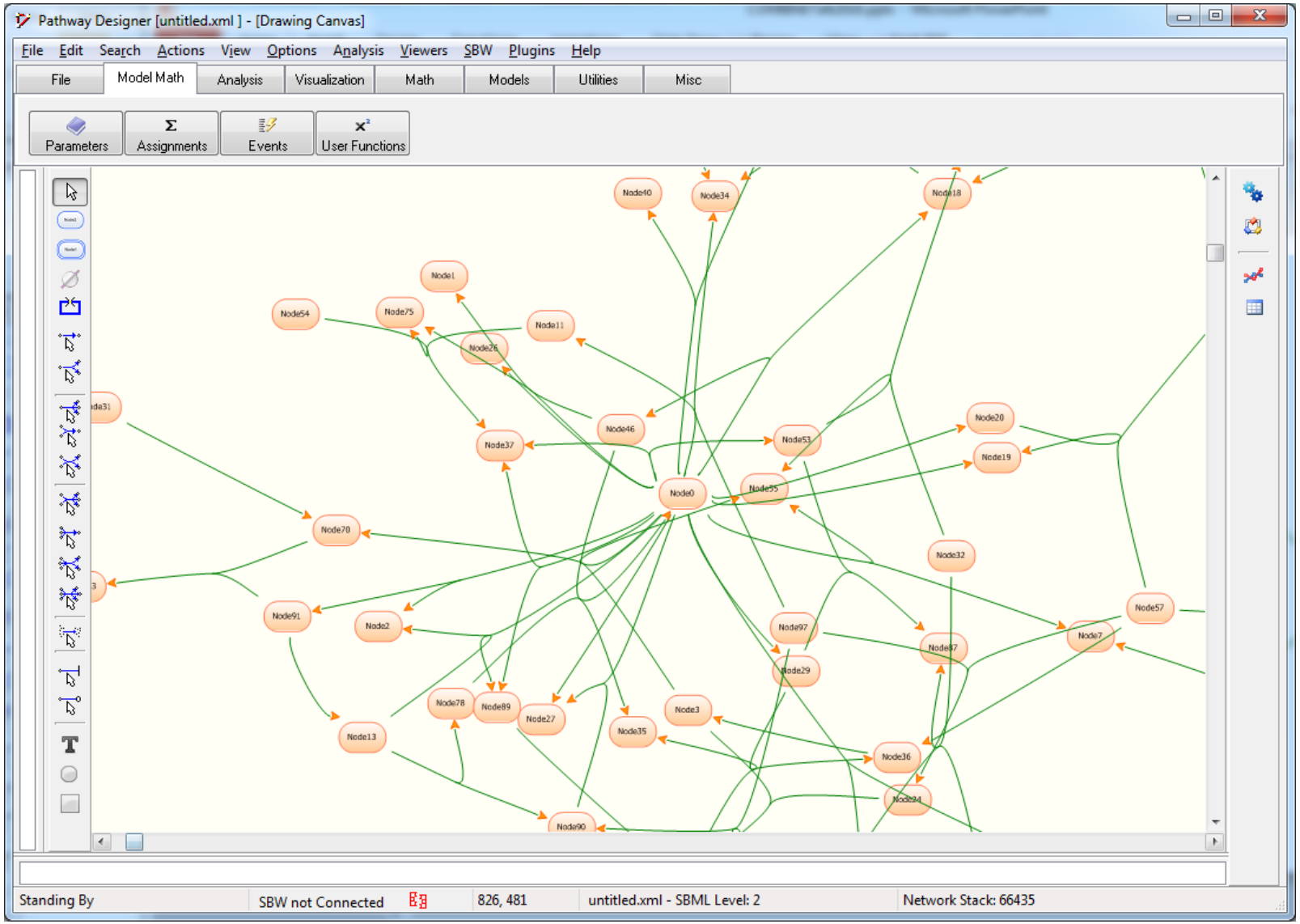


Plugins: AutoLayout, Compartments



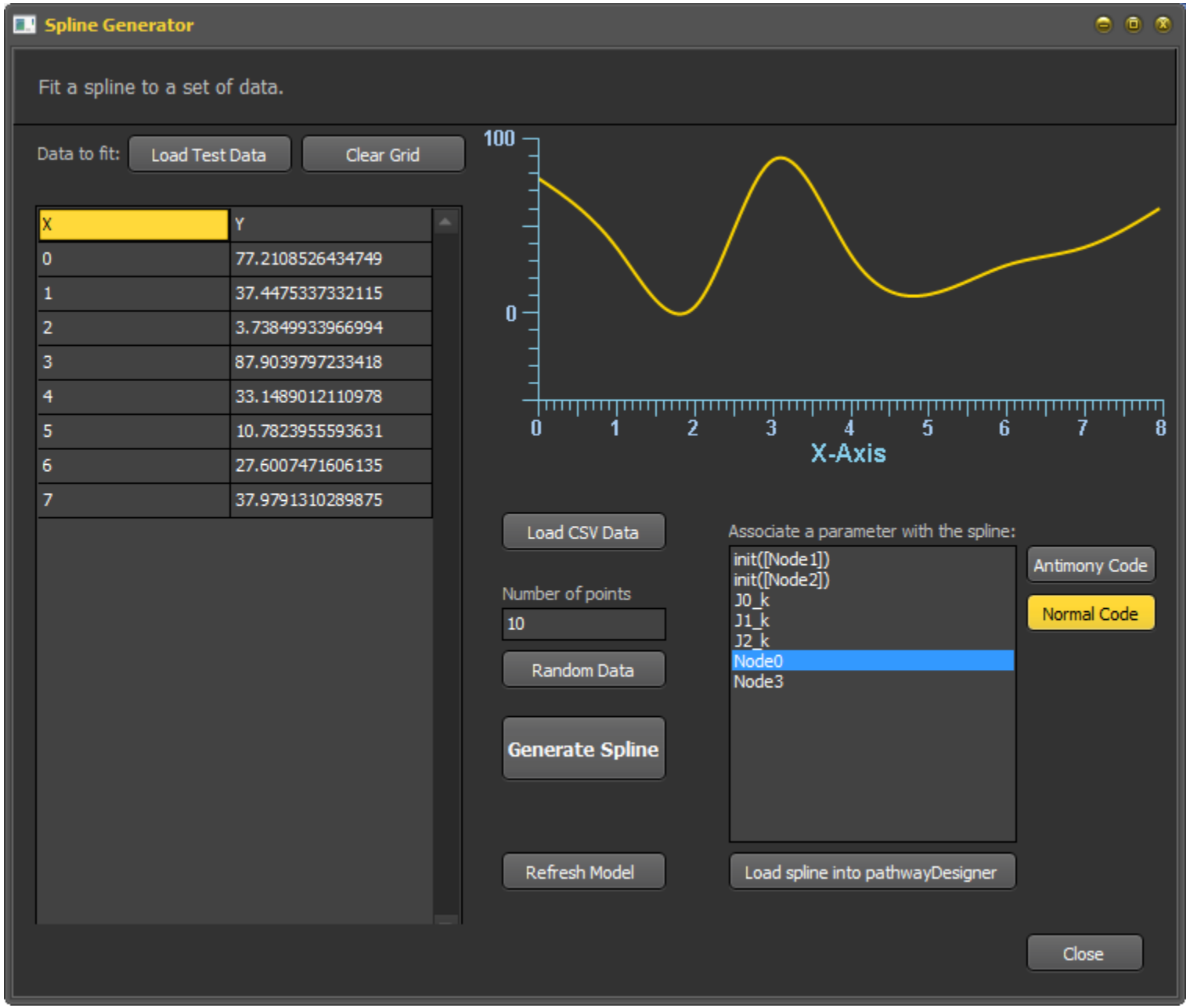


Alias Nodes/Autolayout



Cubic Spline Input

Thanks to Felix Winter

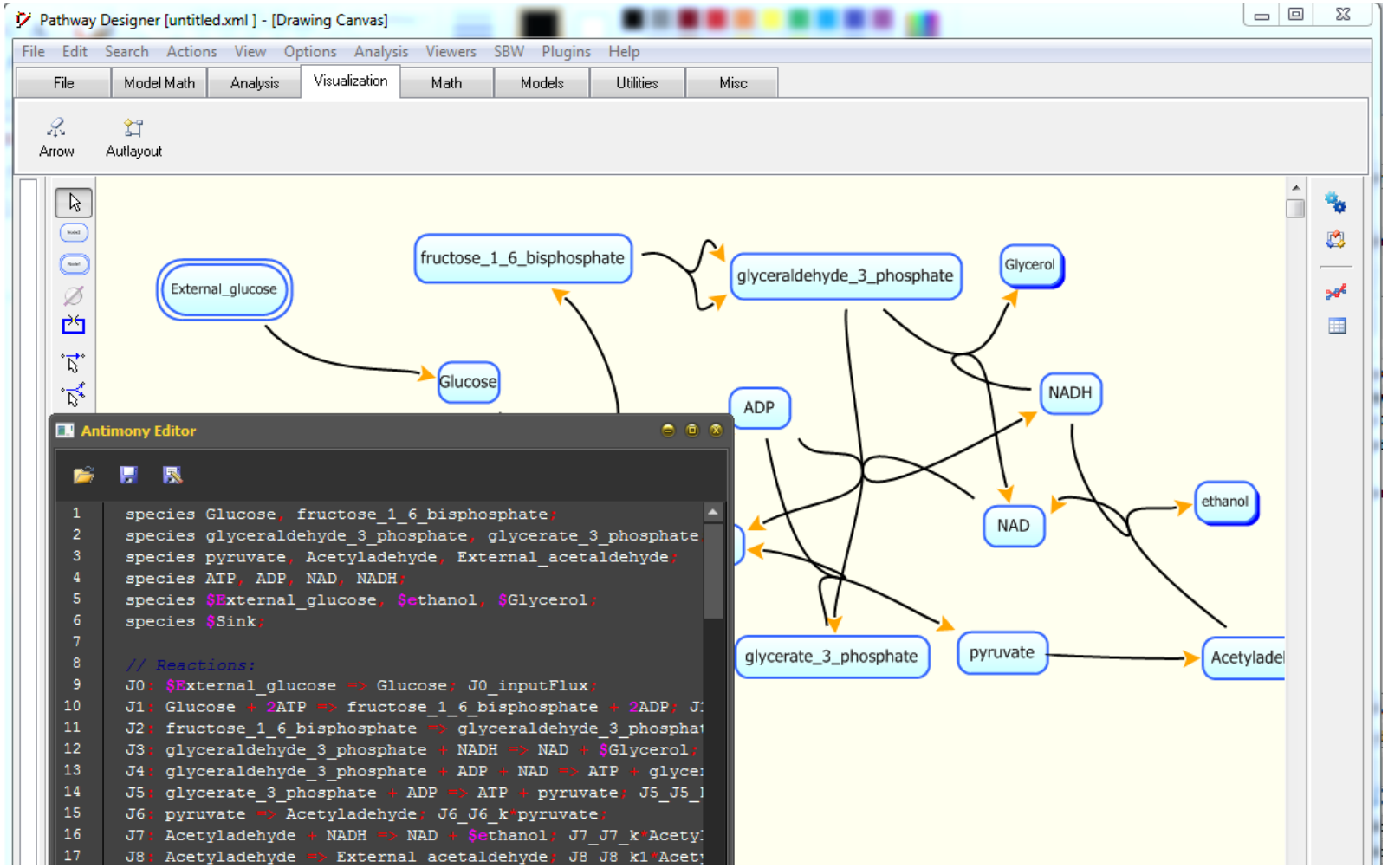


Spline as a piecewise function

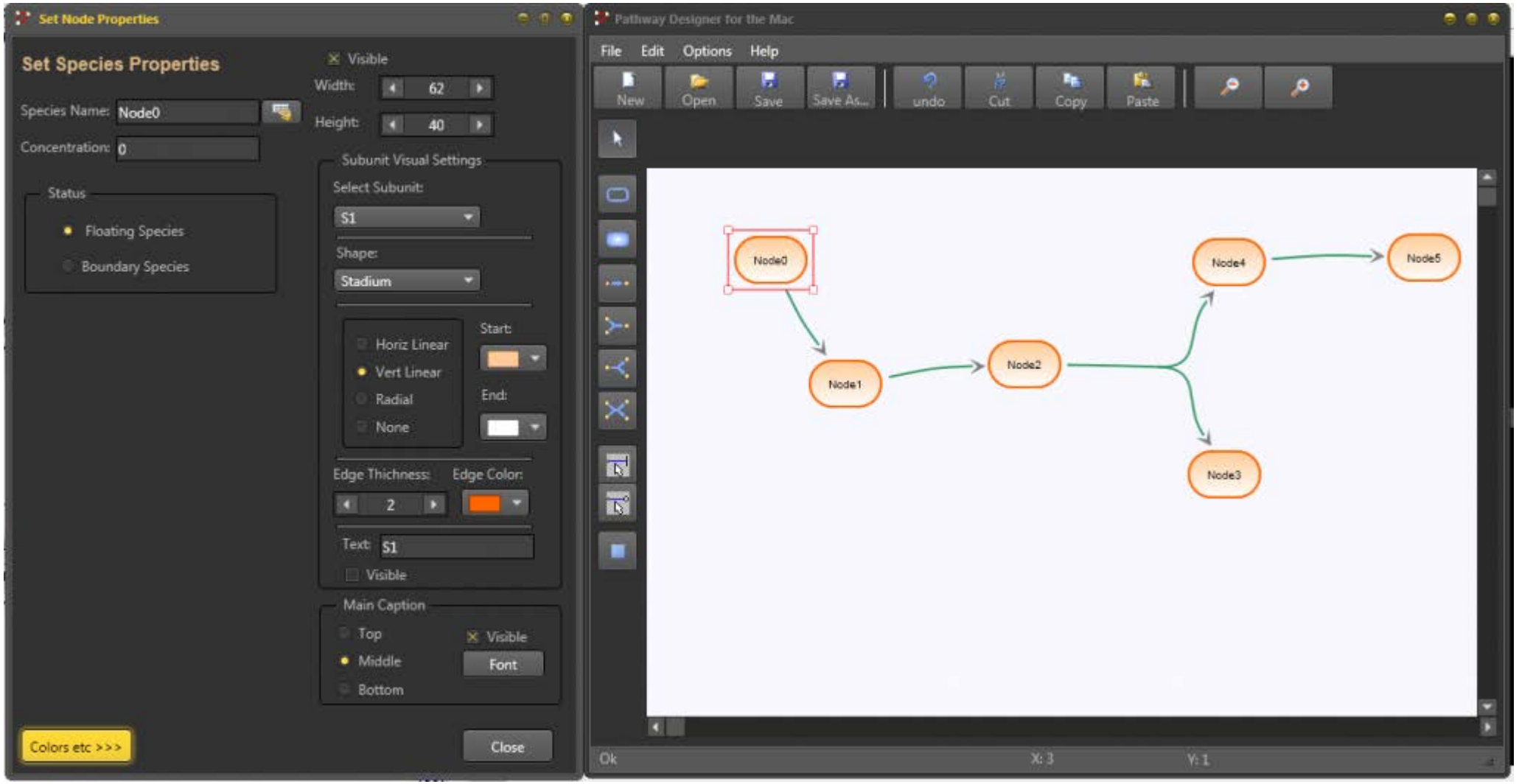
Node0 = piecewise (((-9.622571*(time-0) + 0.000000)*(time-0) - 30.140748)*(time-0) + 77.210853, (time >=0.000000) && (time <= 1.000000), ((54.167142*(time-1) - 28.867714)*(time-1) - 59.008462)*(time-1) + 37.447534, (time >=1.000000) && (time <= 2.000000), ((-95.225764*(time-2) + 133.633710)*(time-2) + 45.757534)*(time-2) + 3.738499, (time >=2.000000) && (time <= 3.000000), ((69.940842*(time-3) - 152.043583)*(time-3) + 27.347662)*(time-3) + 87.903980, (time >=3.000000) && (time <= 4.000000), ((-13.228473*(time-4) + 57.778944)*(time-4) - 66.916977)*(time-4) + 33.148901, (time >=4.000000) && (time <= 5.000000), ((-10.230666*(time-5) + 18.093525)*(time-5) + 8.955493)*(time-5) + 10.782396, (time >=5.000000) && (time <= 6.000000), ((8.526313*(time-6) - 12.598474)*(time-6) + 14.450544)*(time-6) + 27.600747, (time >=6.000000) && (time <= 7.000000), ((-4.326822*(time-7) + 12.980467)*(time-7) + 14.832537)*(time-7) + 37.979131, (time >=7.000000) && (time <= 8.000000))

Pretty!

Plugin: Antimony

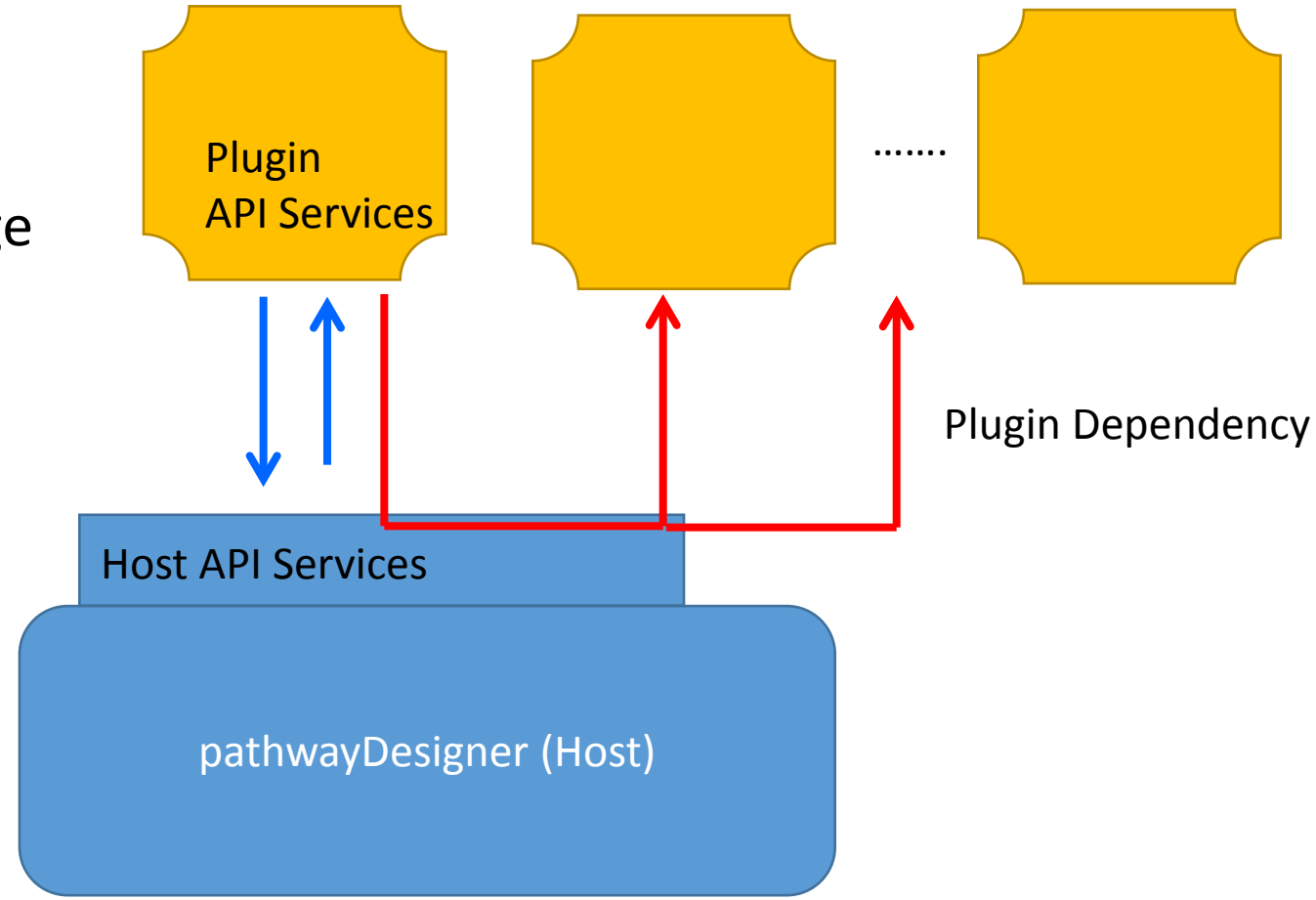


Mac Version – alpha



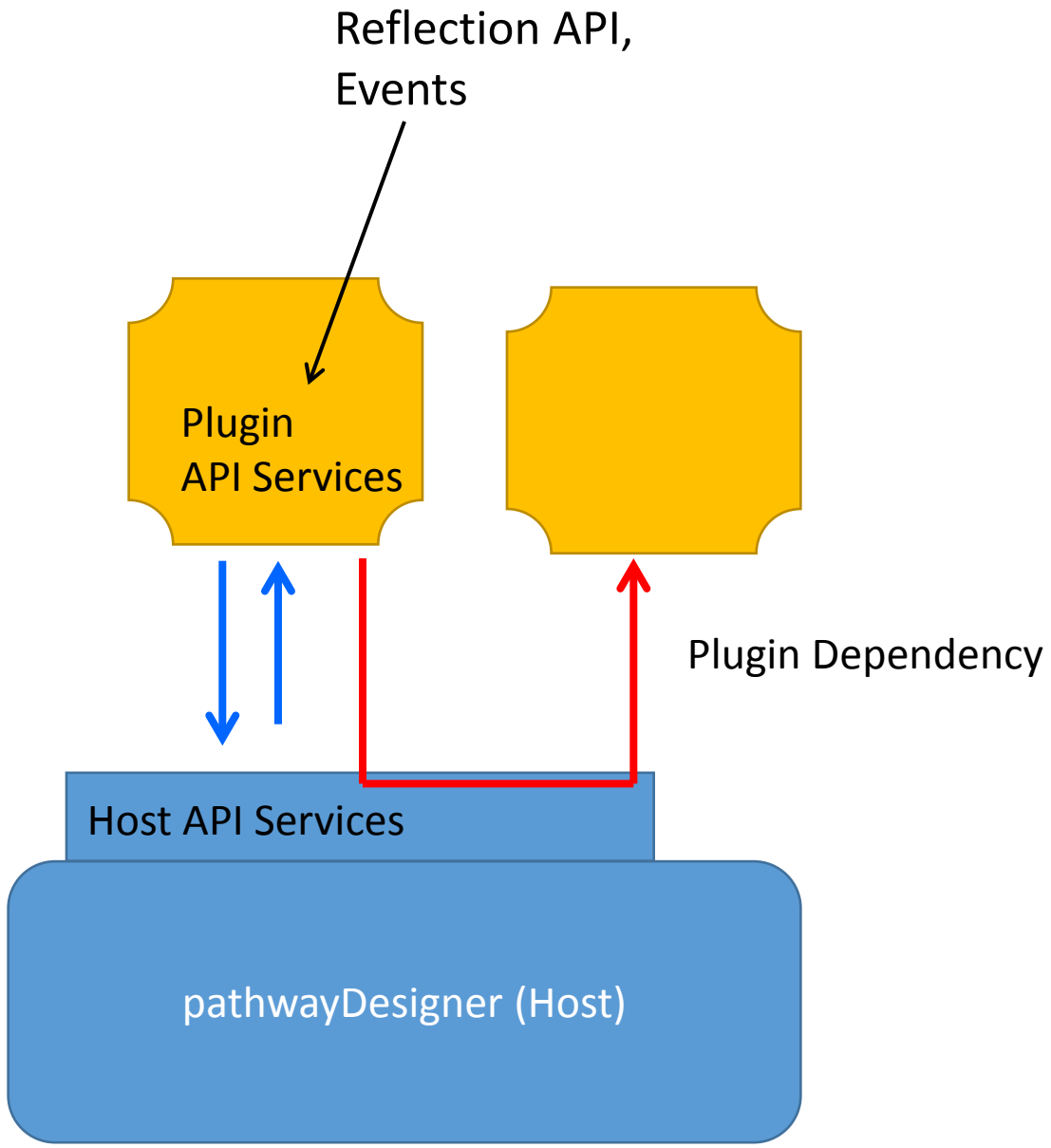
Plugin Architecture

The design is based on the idea that plugins can be written in any language that supports C type calls.

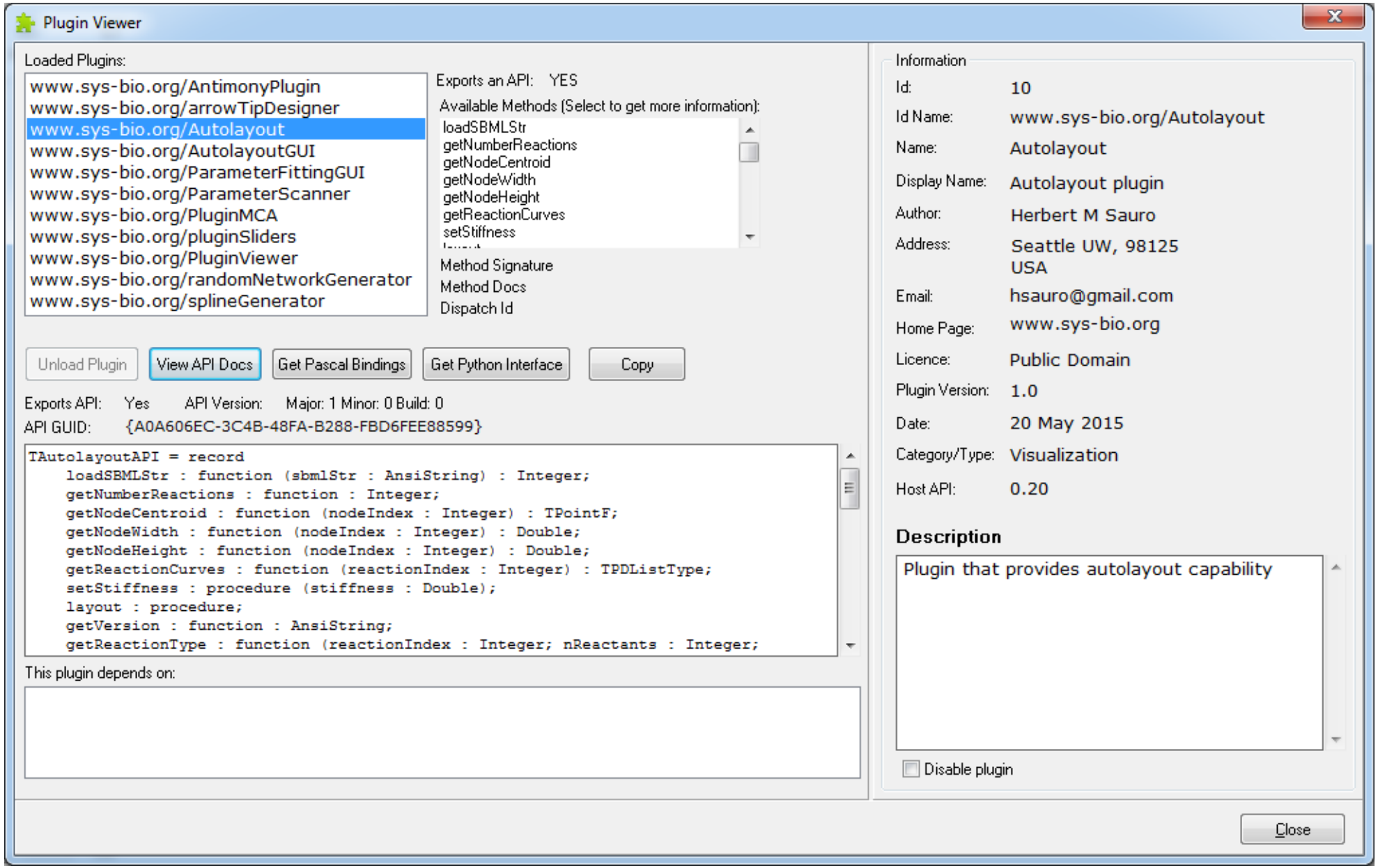


HOST API Services

Utilities
IntegerArray
DoubleArray
StrArray
Matrix – labeled array
List
Network – visual aspects of network
Forms – create GUI components
simulationService – SBW or libRoadRunner
Antimony



Plugin Viewer

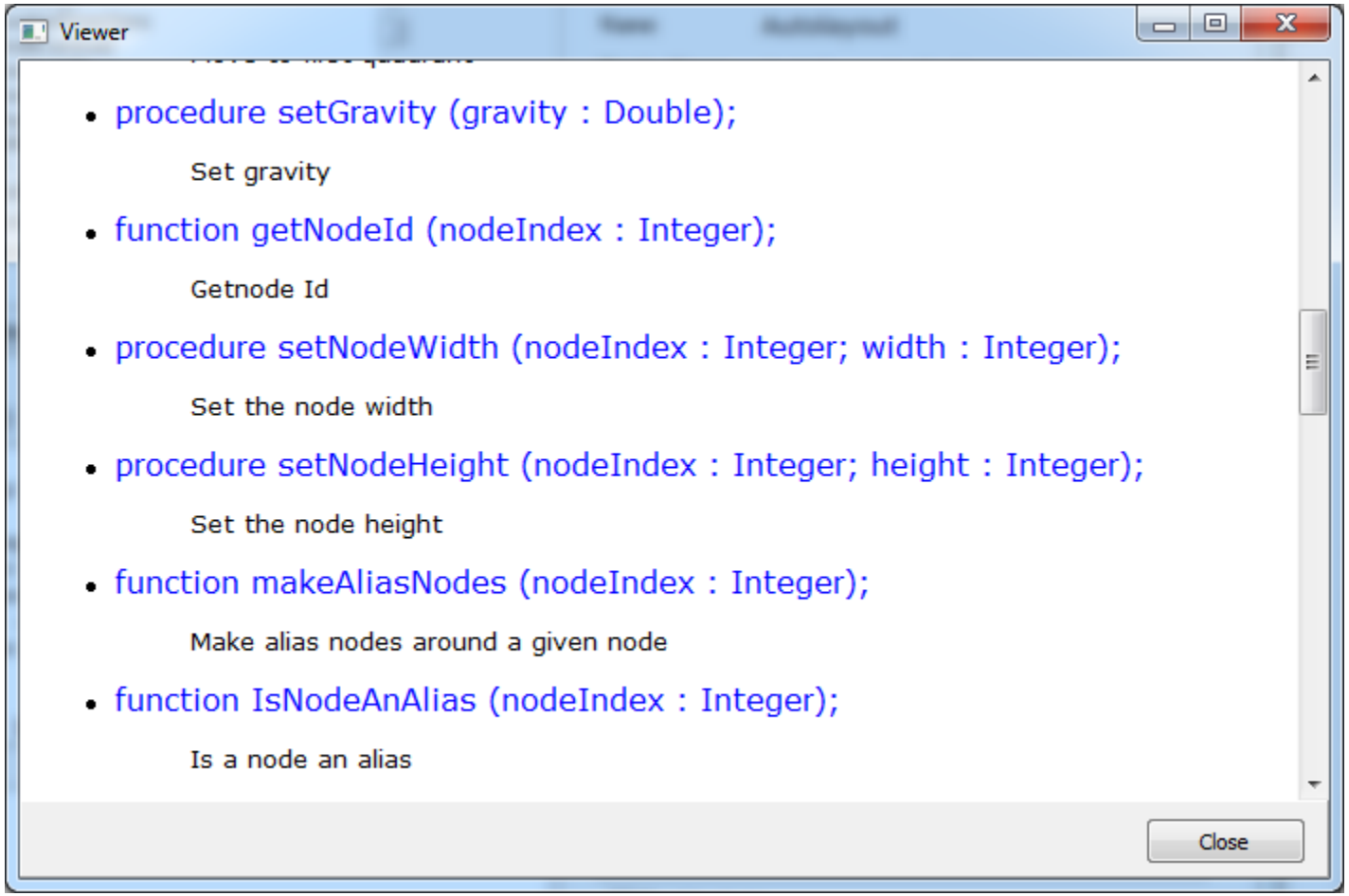


Self Documenting

Reflection API

hasPluginAPI
getAPIGUID
getNumberOfMethodsInAPI
getNameOfMethodInAPI
getNumberOfArgumentsInAPI
getArgumentTypeInAPI
getReturnTypeInAPI
getDocsInAPI
getMethodDispatchIdInAPI

callMethodInAPI



Future

Short Term (within 1 year)
1. Finish the Mac version (single code base for Windows and Mac)
2. Finish support for alias nodes
3. Finish Python plugin
4. Finish saving layouts using layout extension
5. Support render extension?

Long term

Real-tine Interactive simulation

Acknowledgments

Kyle Medley for libSBNW

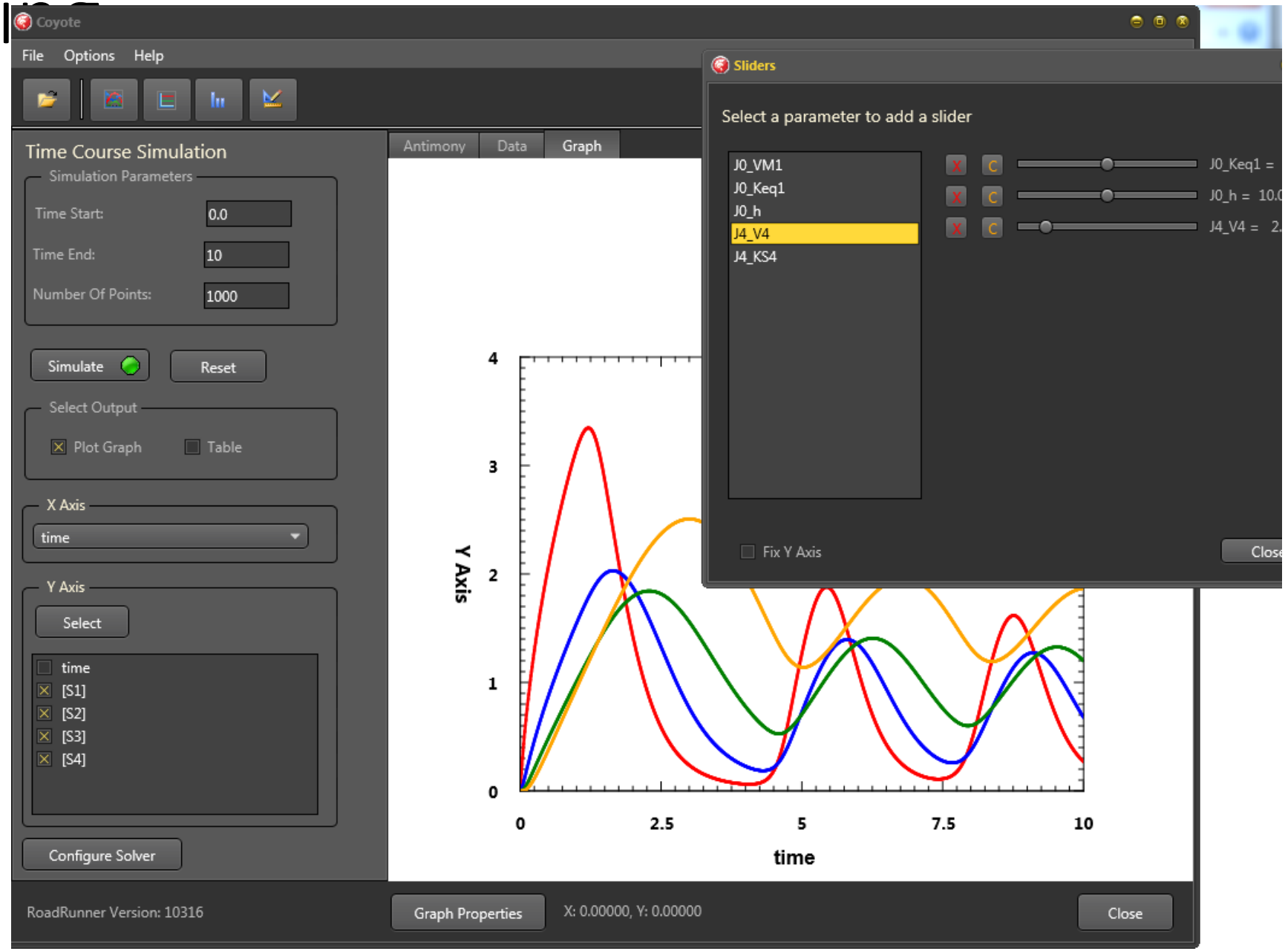
Bosley and Rosa for testing and suggestions

Felix Winter for Cubic Spline ideas

Stackoverflow on how to add borders around triangles

pathwayDesigner.org

Self Documenting



Host Events and Dispatch

OnDestroy
OnBroadcastMessage – message from a plugin to all plugins
OnLoadingComplete
OnModelChange
OnNodeValueChangeByIndex
OnValueChangeById