



JDesigner

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Introduction

- What is JDesigner
- Creating a simple network
- JDesigner Molecule Designer
- JDesigner & SBML Layout
- JDesigner & Simulating SBML
- JDesigner Plans

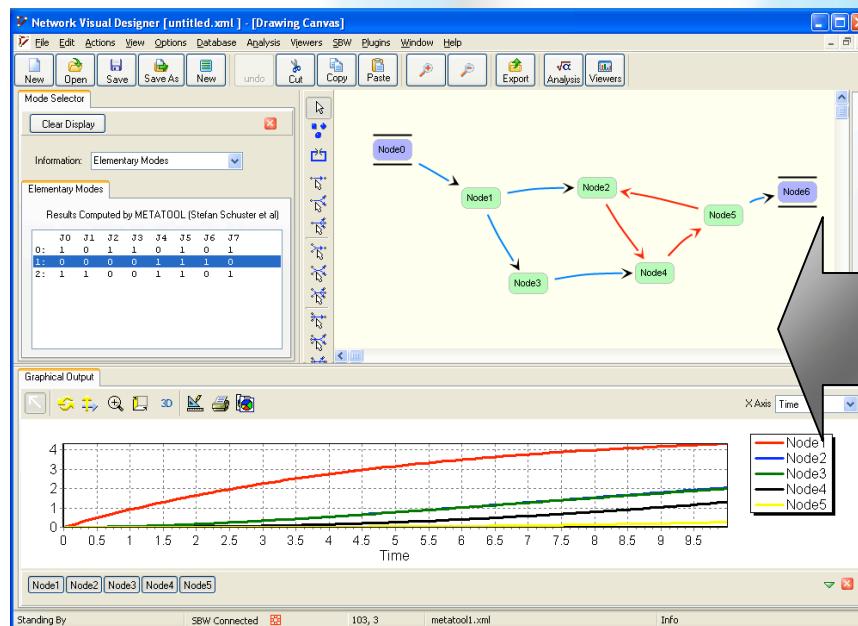
What is JDesigner

- a visual tool for the layout out of reaction networks, including
 - metabolic,
 - signal transduction and
 - gene regulatory networks
- Goals:
 - Provide a simple interface for easy construction and modification of existing networks
 - Allow for analyzing of model with existing tools

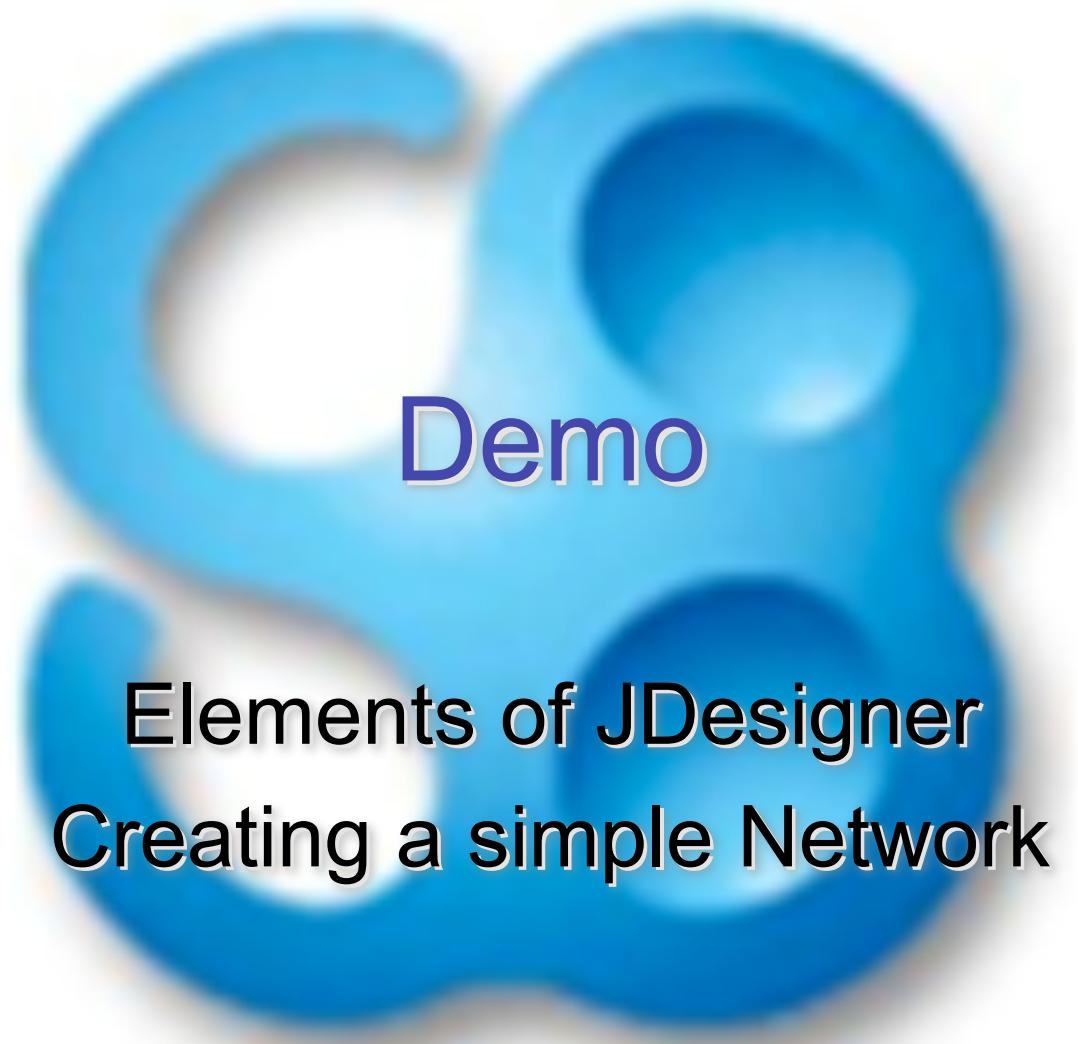
Interaction with other Programs

- JDesigner is tightly integrated into the Systems Biology Workbench (SBW)
 - software infrastructure that:
 - Enables sharing of simulation/ analysis software & models
 - Enables collaboration between software developers
 - SBW:
 - Small API,
 - Simple message-passing architecture
 - Easy to make cross-platform compatible
 - Easy to make distributed:
 - Language neutral architecture:
 - Language bindings for: C/C++, C#, Delphi, Java, Matlab, Perl, Python
 - A registry of services for applications to query

Integration with SBW Simulators:



- e.g. Jarnac
- Analysis Tools:
 - Steady State,
 - Bifurcation Discovery
 - Frequency Analysis
 - Stoichiometry Analysis
 - 3D Concentration Viewer
- SBML as native file format

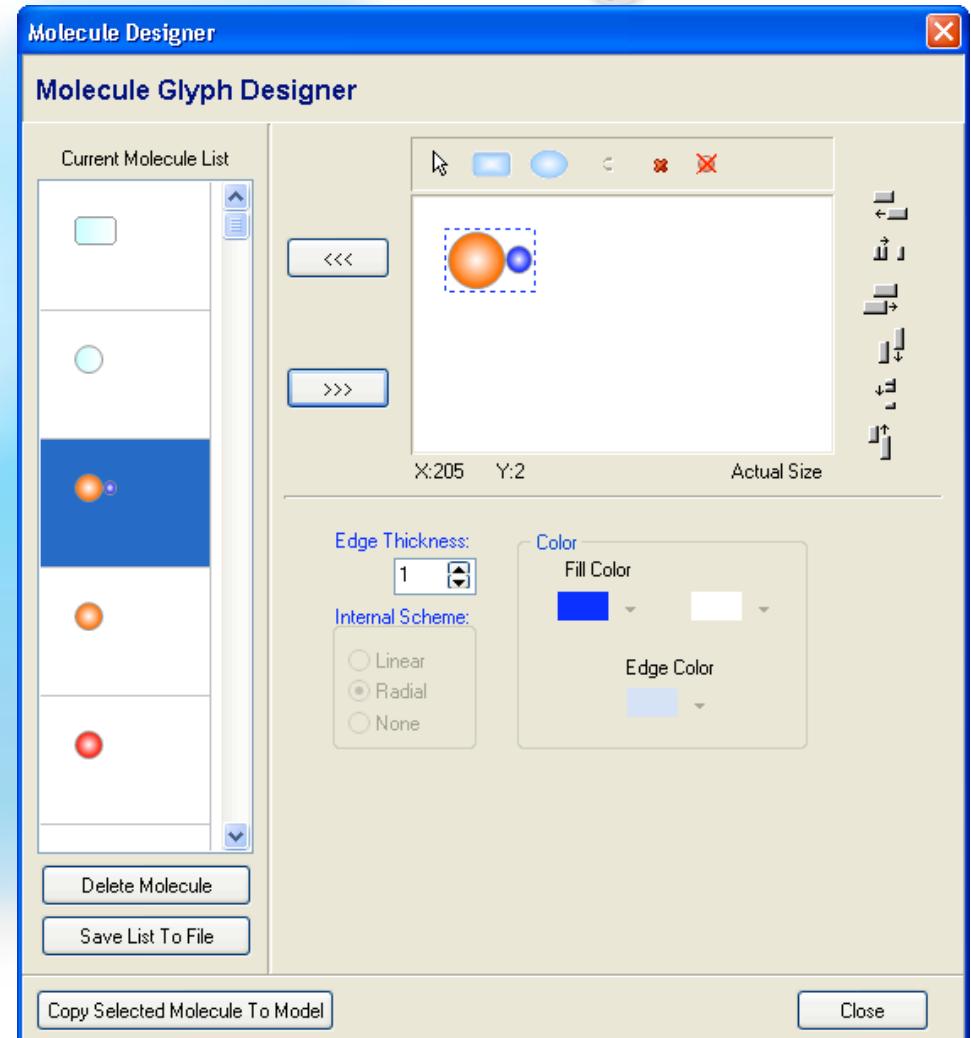


Demo

**Elements of JDesigner
Creating a simple Network**

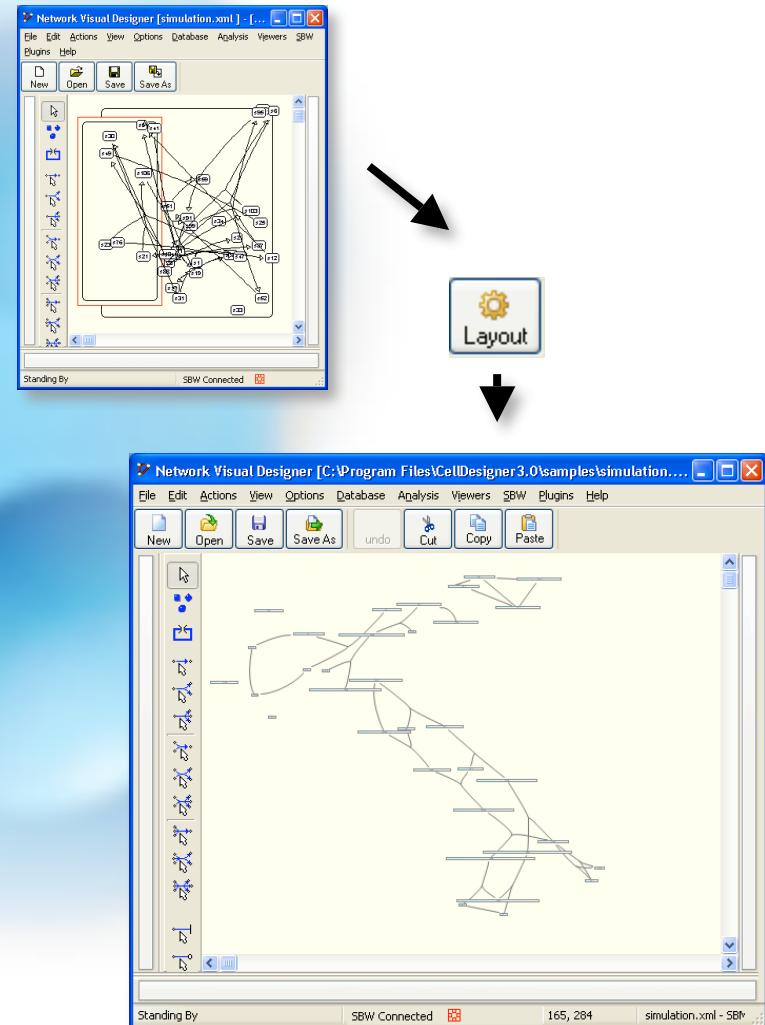
JDesigner Molecule Designer

- JDesigner finally allows specifying complexes and assigning them to species nodes
- Complexes can consist of multiple shapes along with covalent sites
- Note that the changed graphical representation will not modify the simulation
- The so created molecule / complex will be stored for later use
- file format: XML



JDesigner & SBML Layout

- For models without layout annotations a new layout will now be generated in form of the SBML Layout proposal.
 - Additionally the auto layout algorithm can be applied to the currently loaded model.
 - The same auto layout mechanism is also available as standalone & web application.



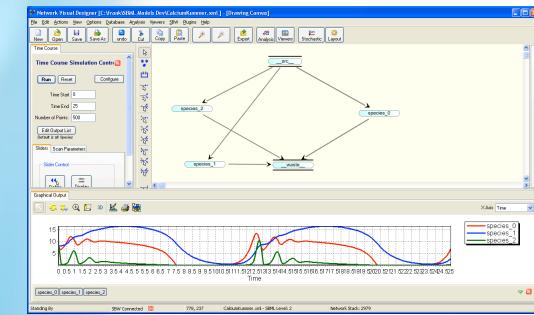


Demo

Auto layout of a Network

JDesigner & Simulating SBML

- It is finally possible to change the SBW simulator that JDesigner uses.
- Supported simulators are currently Jarnac & roadRunner.
- Advantages:
 - roadRunner currently implements most of the SBML Level 2 specification (algebraicRules currently excluded)
 - Speed improvement

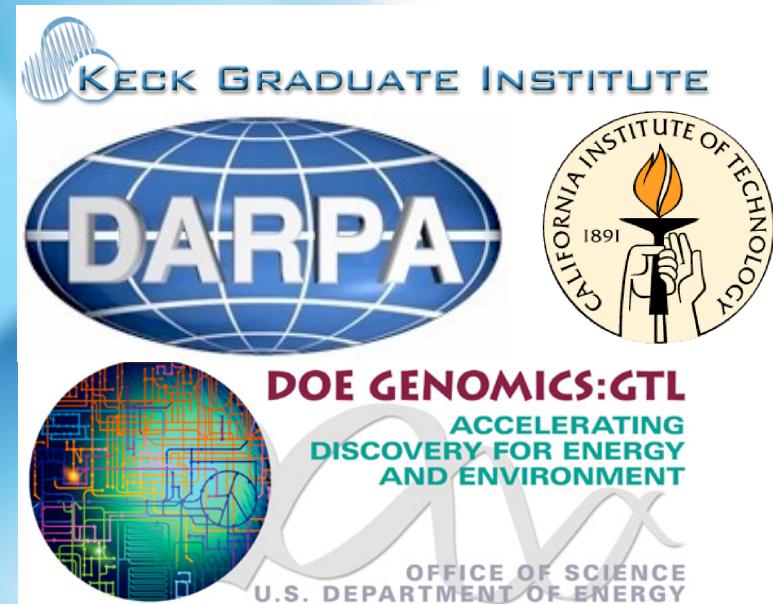


Plans

- Events:
 - Events will be included in JDesigner by adding time & concentration lines.
- Rules:
 - RateRules will be implemented by specifying ODE's for boundary species.

Acknowledgement

- Herbert Sauro, KGI
- Anastasia Deckard, KGI
(work on layout generation)
- Funded through the generous support of ERATO, DARPA (contract number MIPR 03-M296-01) and the DOE (under Grand No. DE-FG02-04ER63804, “Computational Resources for GTL”).
- Original Program Investigators: Hiroaki Kitano, John Doyle, in collaboration with Hamid Bolouri, Andrew Finney and Mike Hucka



More Information

- New Online Tools for :
 - Simulation
 - Validation
 - Translation
 - Renderingof SBML models

<http://www.sys-bio.org>



More Information

- SBML Online Tools:
 - <http://sbw.kgi.edu/Layout/>
 - <http://sbw.kgi.edu/Validate>
 - <http://sbw.kgi.edu/Simulation2005>
 - <http://sbw.kgi.edu/SBMLTranslator>
- SBW
 - <http://www.sys-bio.org>