



KECK GRADUATE INSTITUTE

of Applied Life Sciences

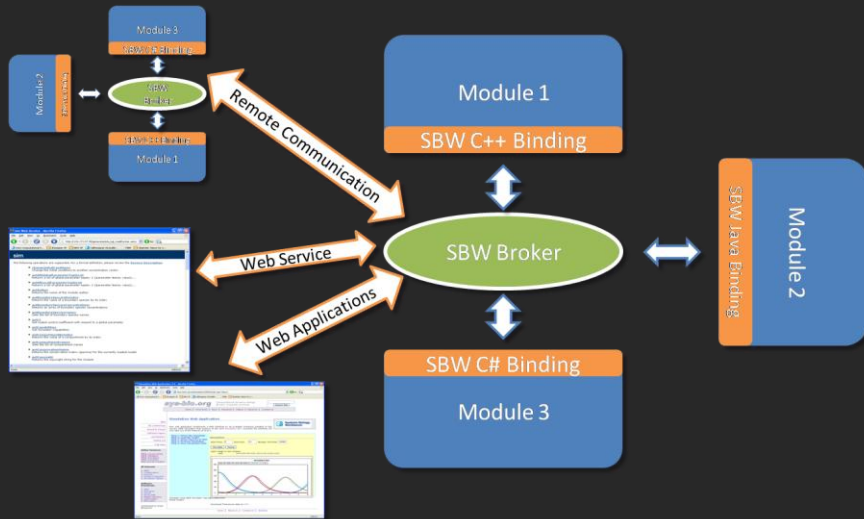


Systems Biology Workbench
Comparing Simulation Results
Structural Analysis & LA library

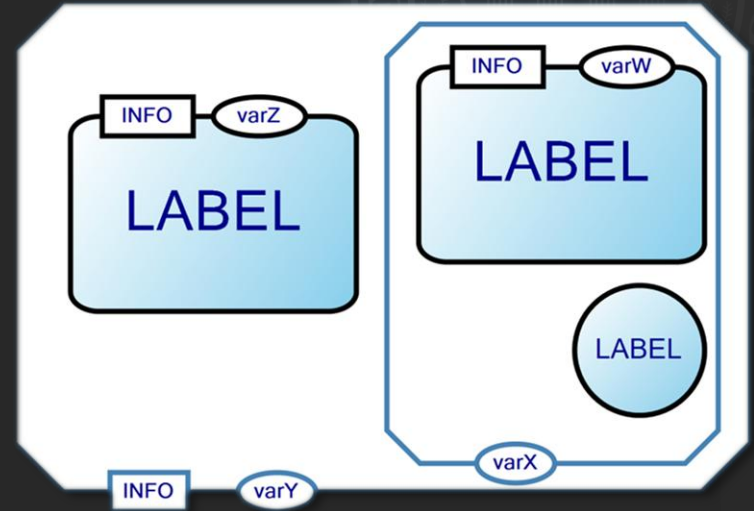
SBW UPDATE

Frank Bergmann (fbergman@u.washington.edu)

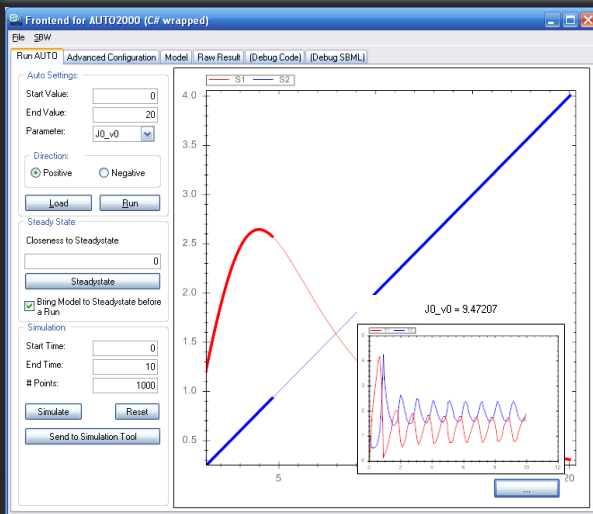
Systems Biology Workbench



Framework Overview



SBGN support



AUTO 2000

SBW Module for Bifurcation Analysis

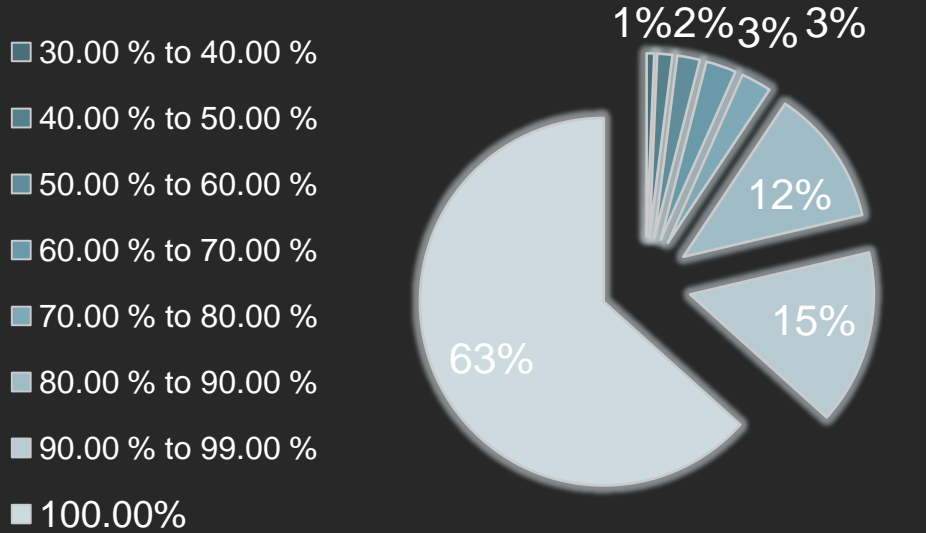
Makes AUTO available from C#

Further updates:

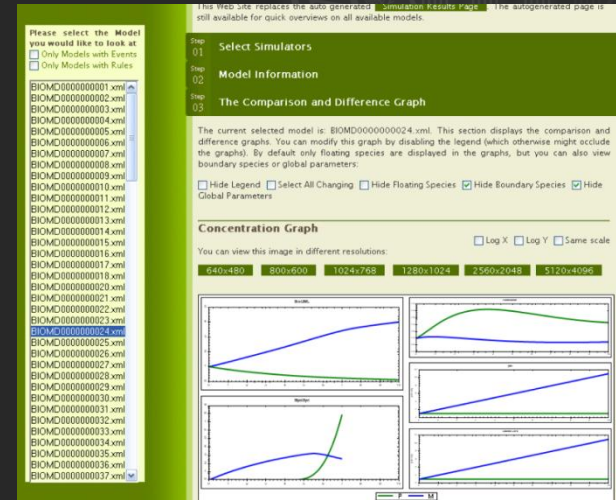
- RoadRunner improvements
- Simulation Tool access to Pulse and Steady State experiments
- MIASE prototype

<http://sys-bio.org>

Comparing Simulation Results



Good news! Most simulators agree!

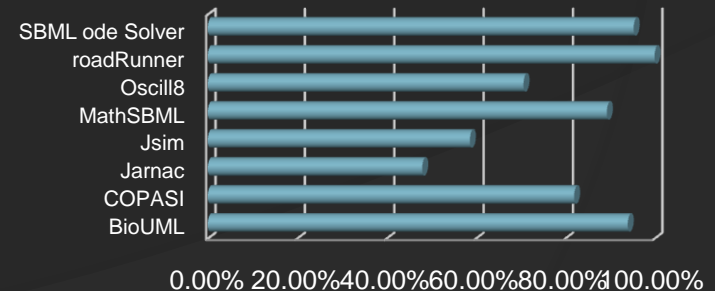


Online Application for analyzing results

The method:

- test across 12 deterministic simulators how well they agree when asked to simulate a given model
- models taken from the BioModels Database

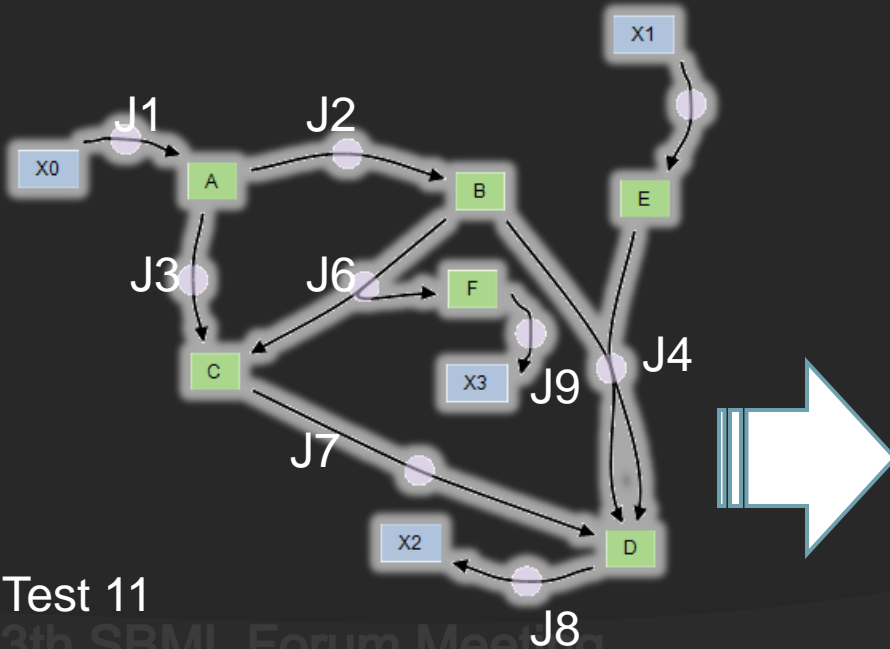
Simulation Results returned for 150 models



Structural Analysis and LA library

Motivation:

- simplify analysis and simulation of biochemical networks by providing a C / C++ / C# library



```

// get matrix to analyze from another part of the code
GetMatrixFromSomeWhere(&oMatrix);

// load it into the structural analysis library
LibStructural_loadStoichiometryMatrix (oMarix, nRows, nCols);

// analyze the stoichiometry matrix using the QR method
LibStructural_analyzeWithQR( &sMessage, &nLength);

// print model overview
printf("%s", sMessage);

// free the memory used by the message
LibStructural_freeVector(sMessage);

// obtain and print the test results
LibStructural_getTestDetails( &sMessage, &nLength );

// finally free the memory used by the message
LibStructural_freeVector(sMessage);
  
```

Steady State Analysis (non-singular Jacobian)
 Conservation Analysis (L, L0 Matrices)
 Flux Balance Analysis (K, K0 Matrices)

<http://sys-bio.org/fbergman/libstructural>

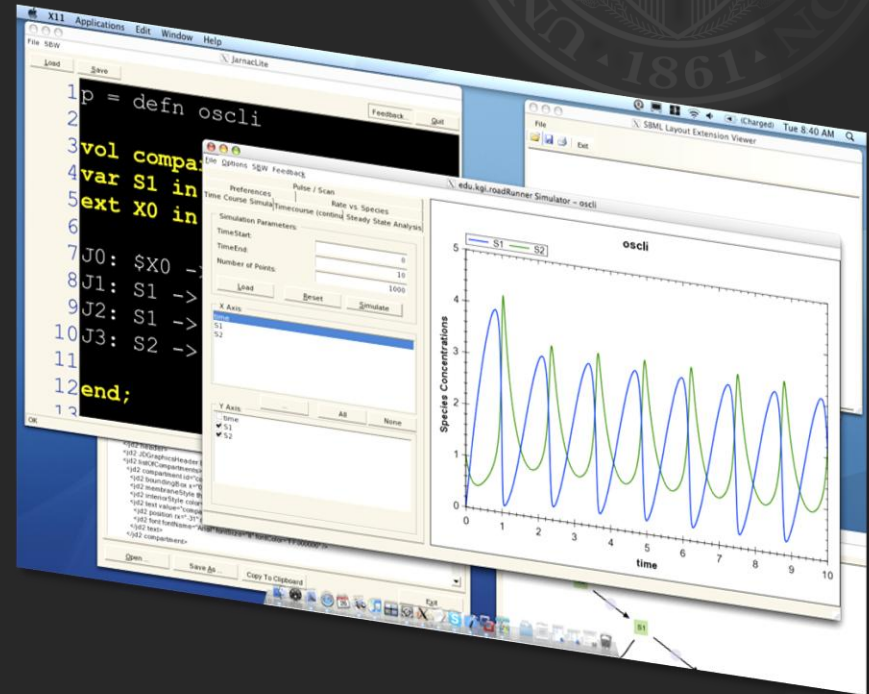
SBW 2.7.8 Release

Non-Windows Release

- Model Creation Editing via JarnacLite
- Simulation via RoadRunner & Simulation Tool
- Layout through Layout Generation Tool

Windows Release

- Jarnac updates for stochastic Simulation / Analysis



Acknowledgements

KGI:

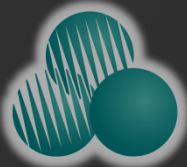
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Thank You !

<http://sys-bio.org>