

KECK GRADUATE INSTITUTE
of Applied Life Sciences



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COMPARING SIMULATION RESULTS

Motivation

- ⦿ Simulations are an essential tool when analyzing biochemical networks.
- ⦿ Researchers and developers seeking to refine simulation tools or develop new ones would benefit greatly from being able to compare their simulation results



The Problem

- With SBML we have a complex MDL for storing computational models
- Many simulation tools for SBML exist
 - Each with its own strength and weaknesses (which might not even be apparent to users (and developers))



The Solution (?)

Having a set of simulation results obtained from a set of well curated models, covering a large subset of SBMLs features would provide a way to test those simulation packages

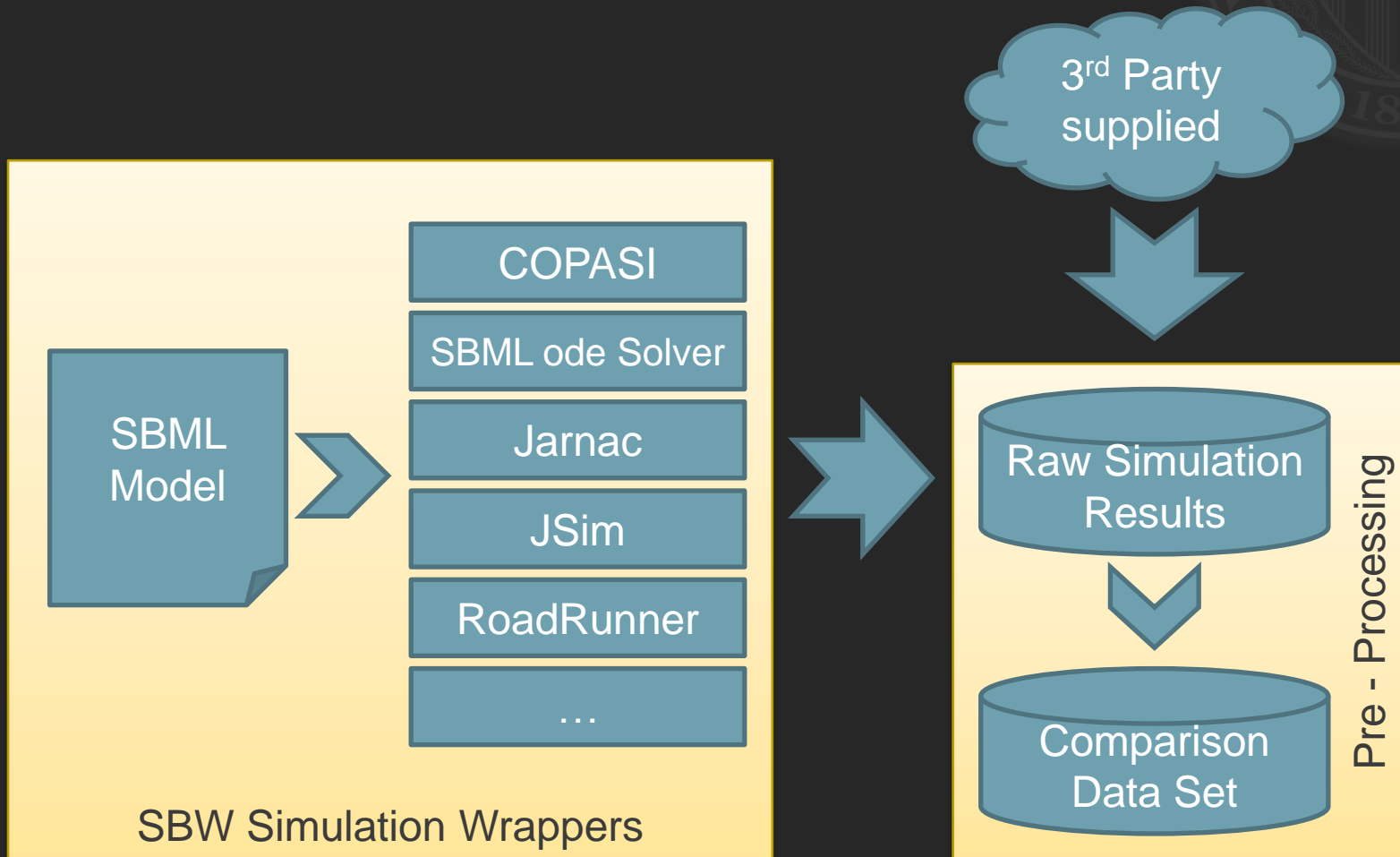
→ No such set of simulation results exists.

Approach

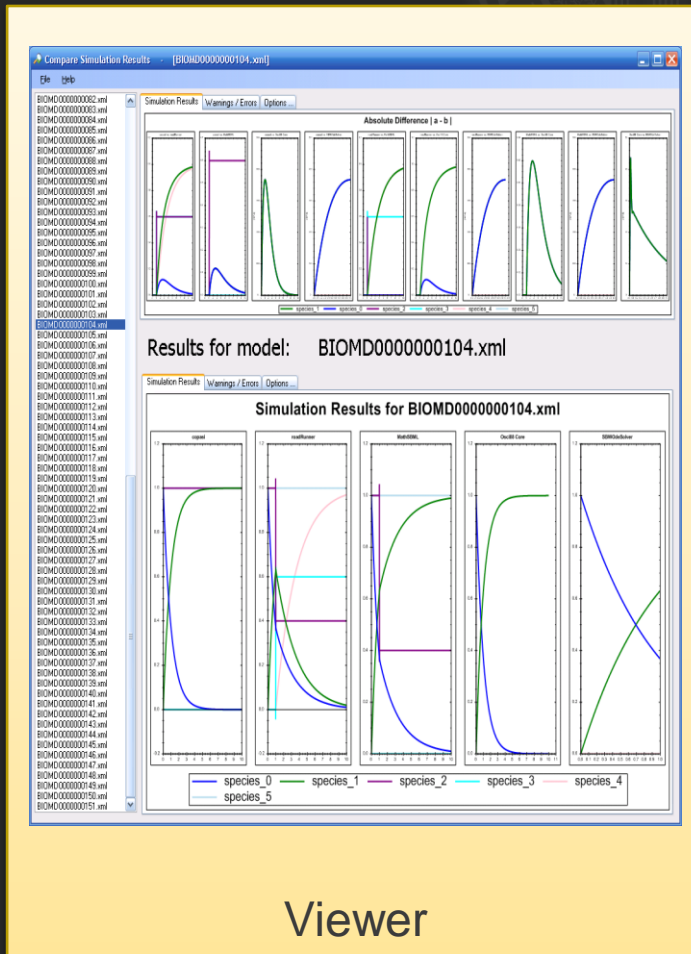
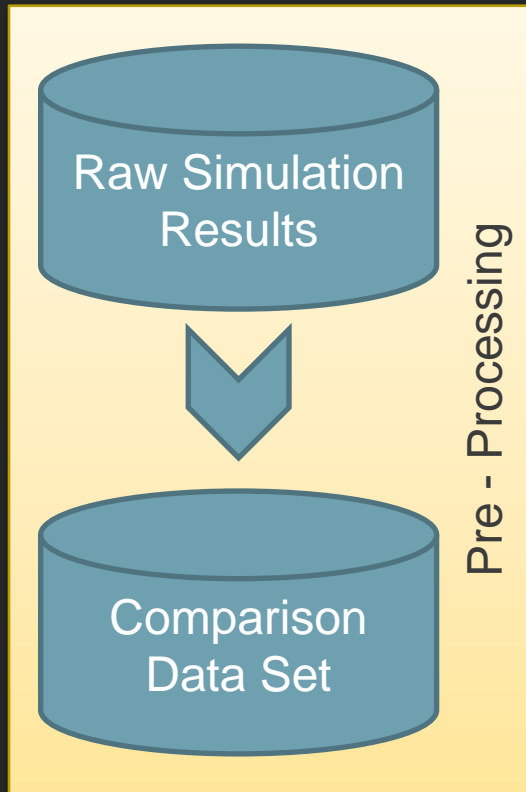
- ⦿ Set of curated models:
<http://biomodels.net>
- ⦿ Representative set of today's simulators:
 - COPASI
 - Jarnac
 - roadRunner
 - SBML ode Solver (SOS lib)
- ⦿ Let them all solve the same problem and see what will happen.



What actually happens

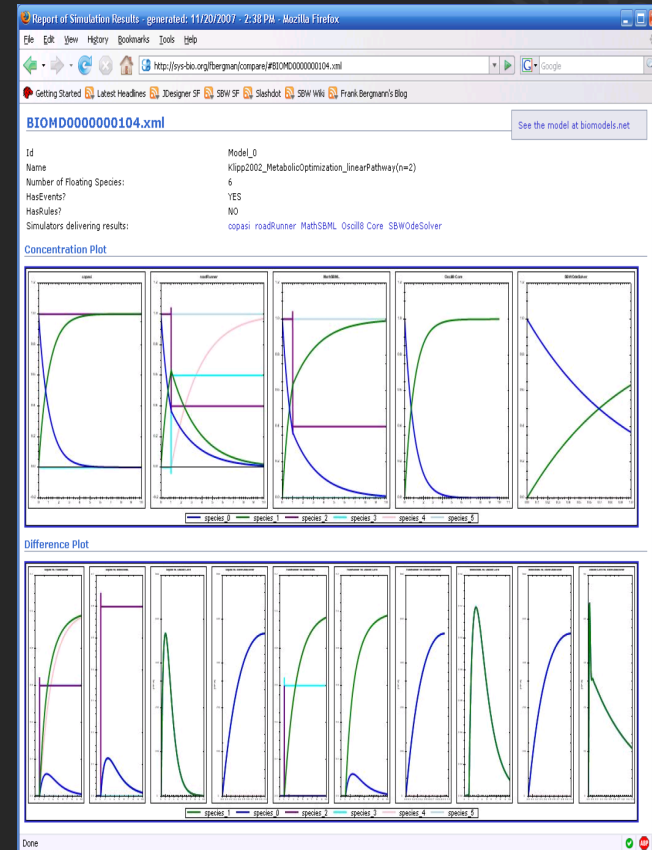
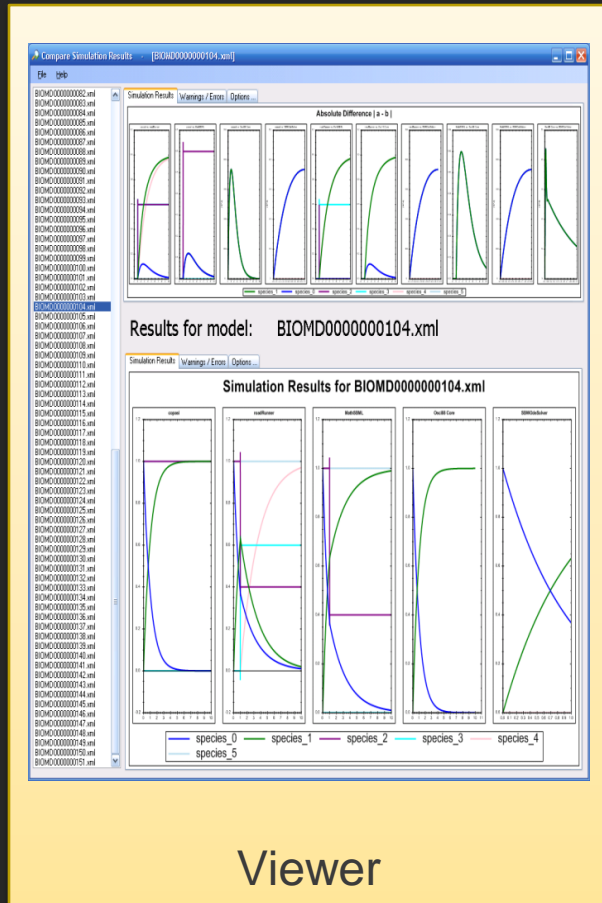


What actually happens



What actually happens

Comparison Report

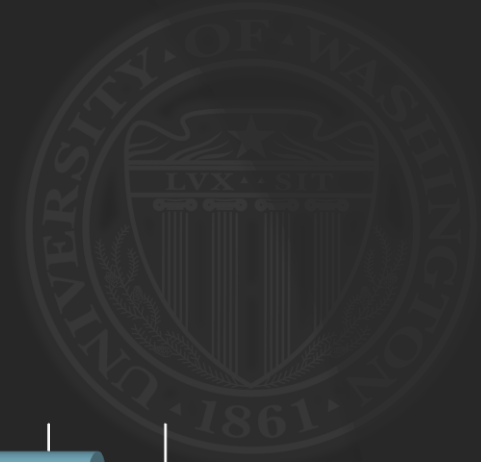


The Results

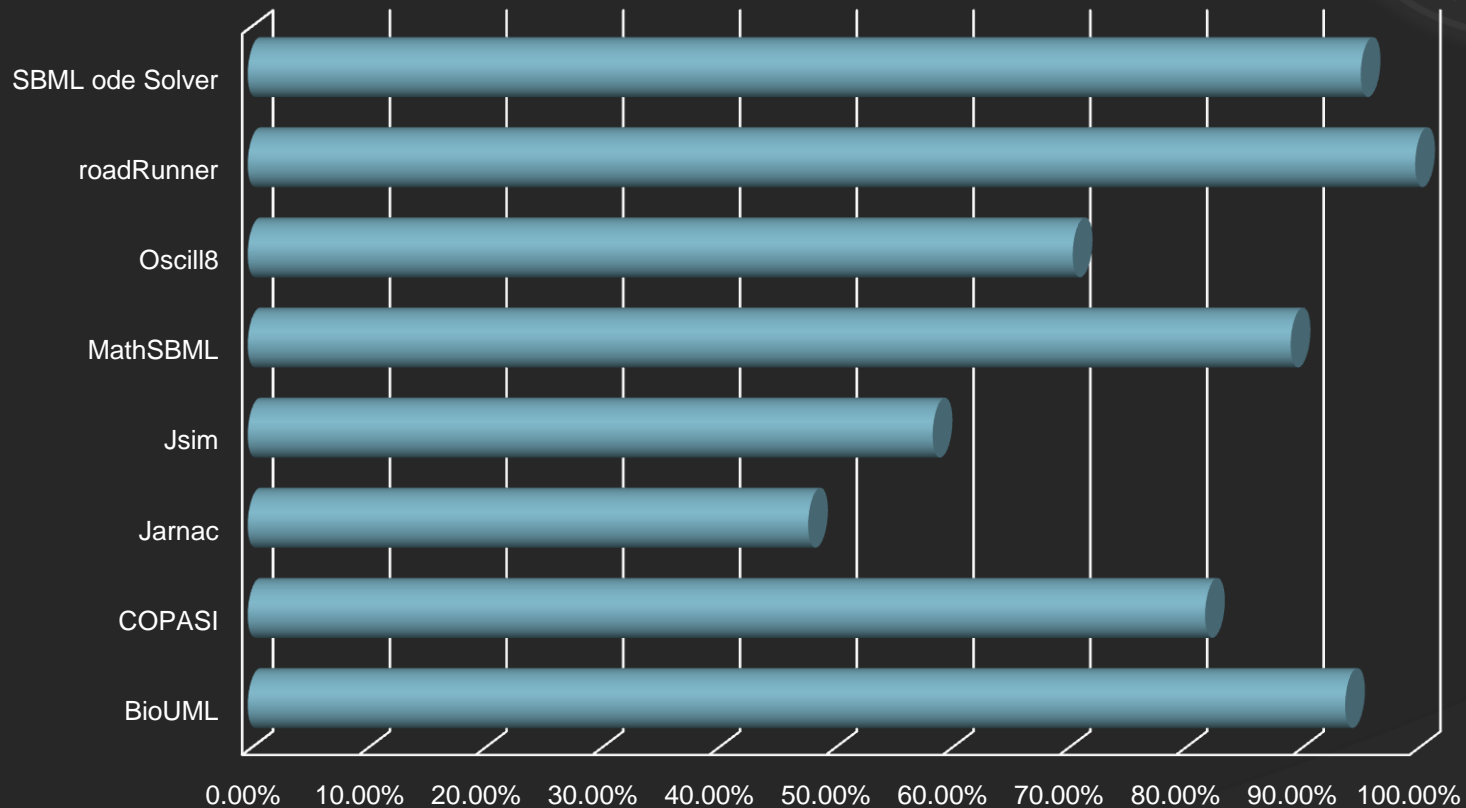
- ⦿ Wrapped Simulators:
 - COPASI
 - Jarnac
 - JSim
 - Oscill8
 - roadRunner
 - SBML ode Solver
- ⦿ Submitted Results
 - MathSBML
 - BioUML
 - ...



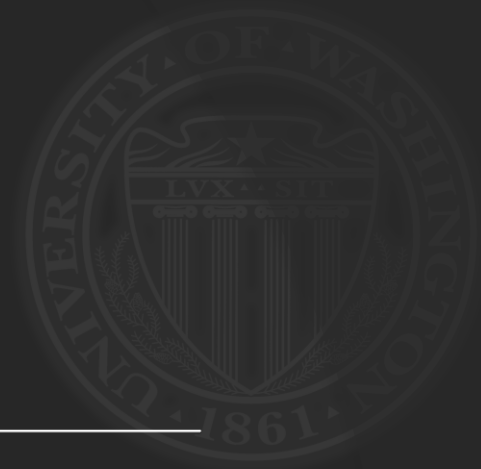
The Results



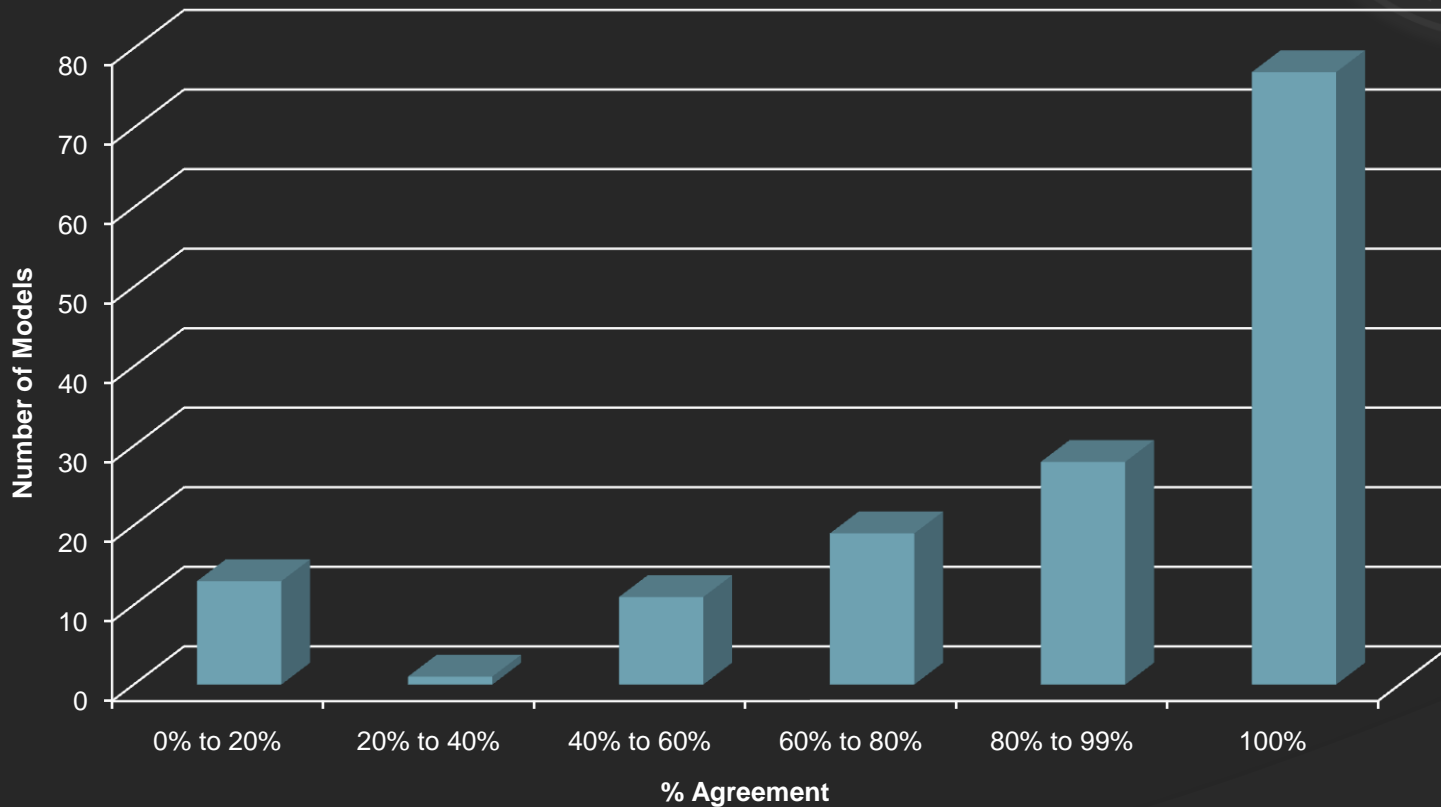
Simulation Results returned for 150 models



The Results

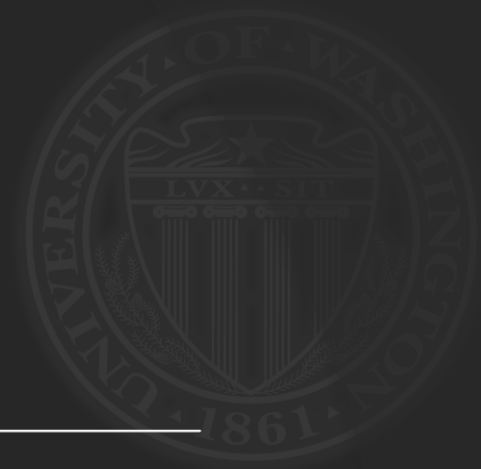


% Agreement of Simulation Results

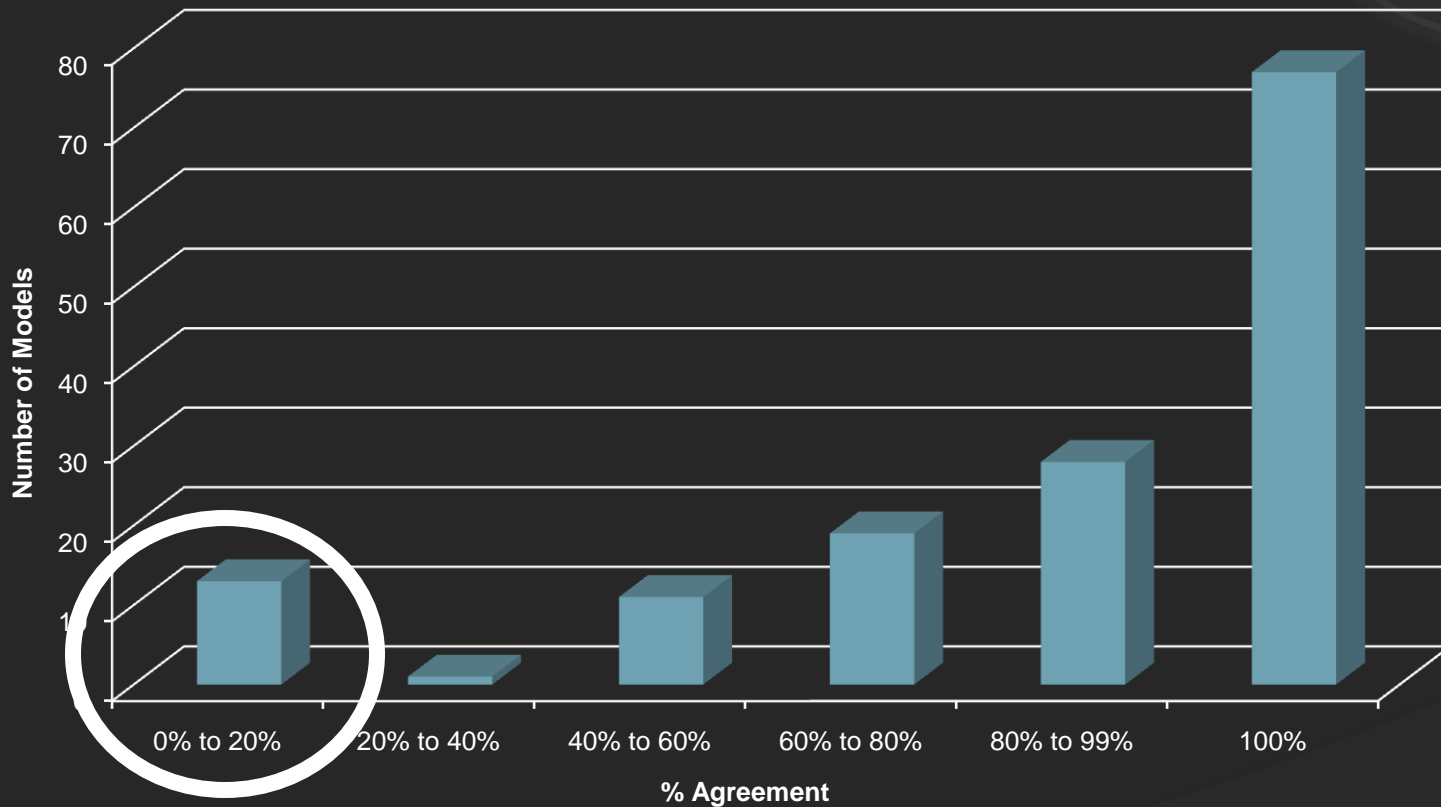


(BioUML results not included in this graph)

The Results



% Agreement of Simulation Results



(BioUML results not included in this graph)

The

Report of Simulation Results - generated: 11/20/2007 - 2:38 PM - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://sys-bio.org/fbergman/compare/#BIOMD0000000104.xml

Getting Started Latest Headlines JDesigner SF SBW SF Slashdot SBW Wiki Frank Bergmann's Blog

BIOMD0000000104.xml

[See the model at biomodels.net](#)

Id: Model_0
Name: Klipp2002_MetabolicOptimization_linearPathway(n=2)
Number of Floating Species: 6
HasEvents?: YES
HasRules?: NO
Simulators delivering results: copasi roadRunner MathSBML Oscill8 Core SBWOdeSolver

Concentration Plot

Difference Plot

Number of Models

ph)

Outlook

- ⦿ Update results / Add YOUR results
- ⦿ Provide some statistics
 - Comparing Relative / Absolute Difference is not sufficient !!!
- ⦿ Push MIASE / KiSAO !!!



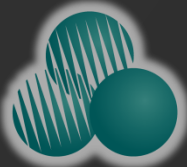
Funding

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Thank You!

<http://sys-bio.org>

<http://sys-bio.org/sbwWiki/compare>