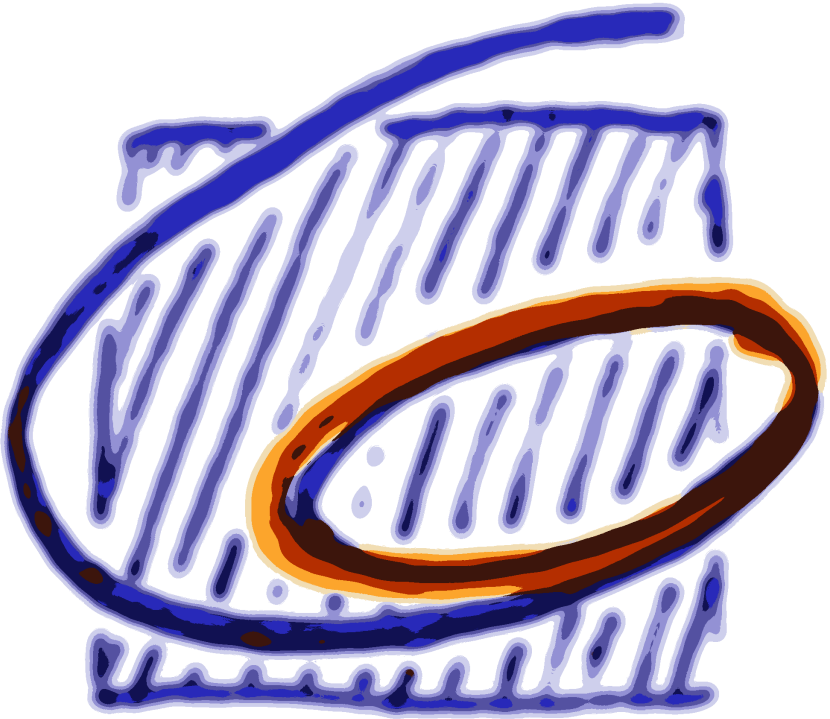
COPASI

Complex Pathway Simulator



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COS Heidelberg / BIOQUANT
Abt. Modellierung biologischer Prozesse

BioQuant
MODEL base of LIFE

General info about COPASI

COPASI is a software tool for editing, simulating, and analyzing quantitative models of biochemical reaction networks.

COPASI is available for all major platforms (**Linux, Windows, OS X**), easy to install

COPASI is free software.

General info (continued)

COPASI is a joint project of the groups of Ursula Kummer (Heidelberg) and Pedro Mendes (Blacksburg, VA and Manchester)

COPASI is designed to be robust and user friendly, intended for general use not only by experts

Download from **www.copasi.org**

Checking models

COPASI can identify some common sources of problems with biochemical models.

Example: A reaction is marked as irreversible but its rate is not zero when a substrate is missing.

This is done by symbolic analysis of the kinetic functions.

SBML support

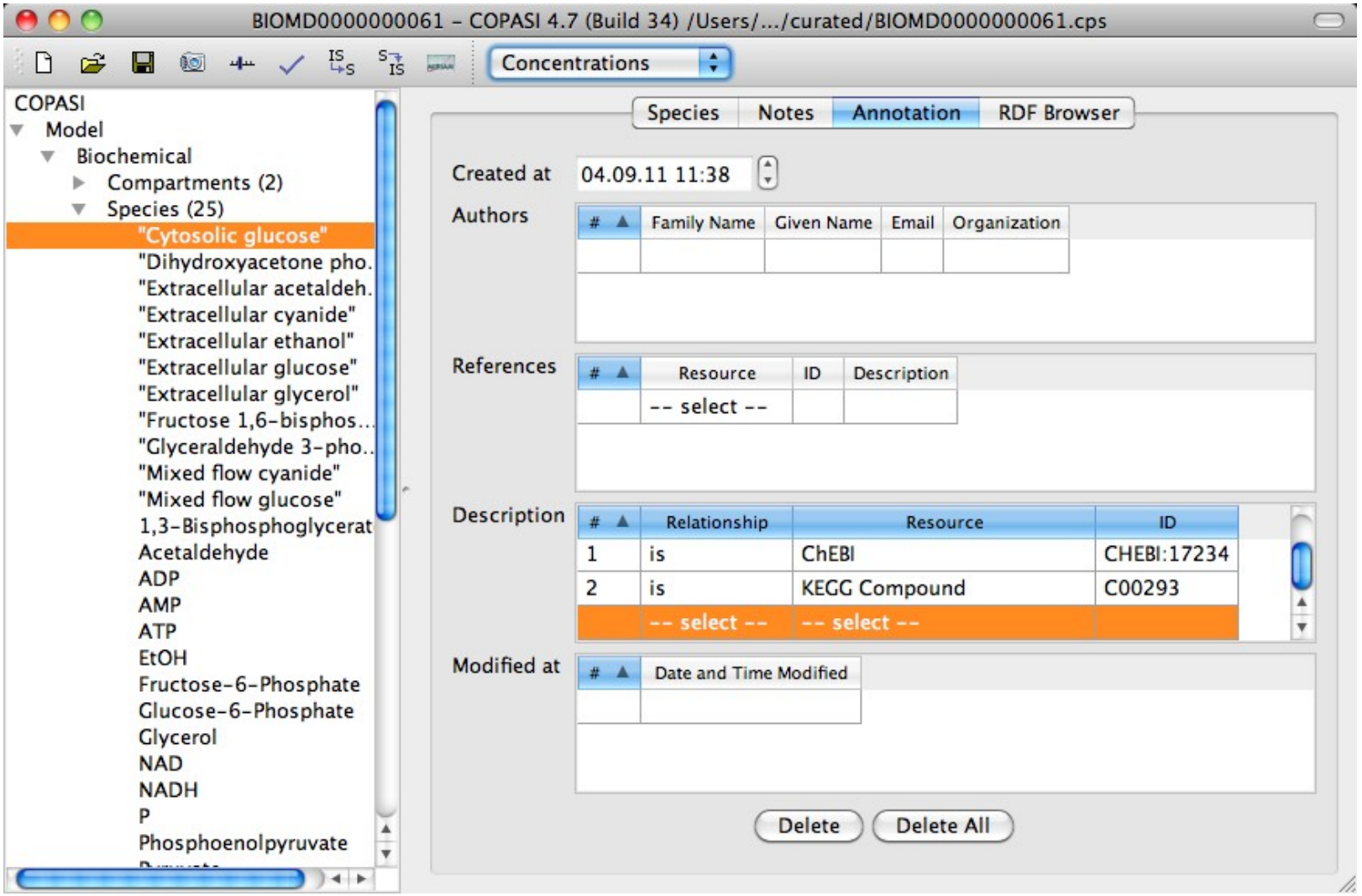
SBML is an XML file format to exchange biochemical models between different tools.

www.sbml.org

COPASI implements a large subset of the SBML specification. SBML complience is well tested. The COPASI team is actively involved in the development of SBML

MIRIAM annotations

Editing and display of annotations is supported.



different mathematical interpretations of a model

A key feature is the ability to switch transparently between a deterministic and a stochastic model interpretation

- Deterministic: ODEs are automatically generated and solved using LSODA

- Stochastic: Reaction rates are converted to reaction probabilities. Exact simulation with Gibson/Bruck or hybrid simulation

Steady State analysis

- Robust algorithm to find steady states
- Stability analysis (eigenvalues of jacobian)
- Metabolic control analysis / MCA (control coefficients)

Structural analysis

- Identification of conservation relations

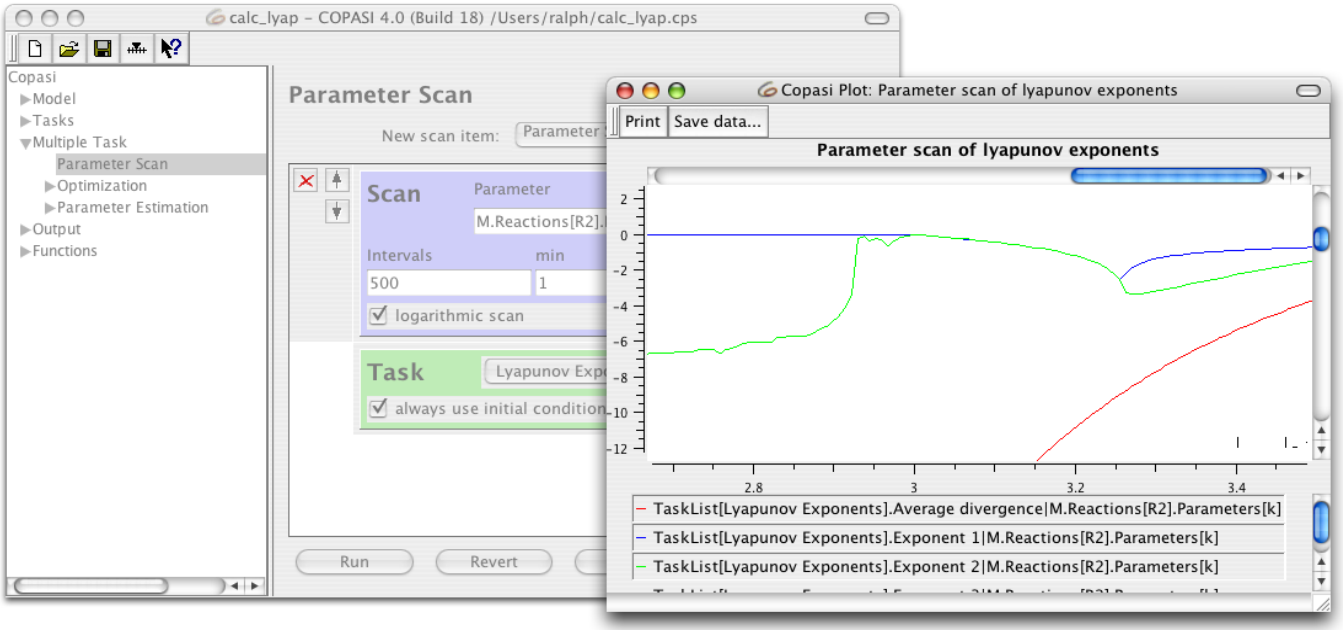
  A + E <-> AE -> B E + AE is conserved

  Very efficient and exact algorithm (Householder method)

- Elementary flux modes

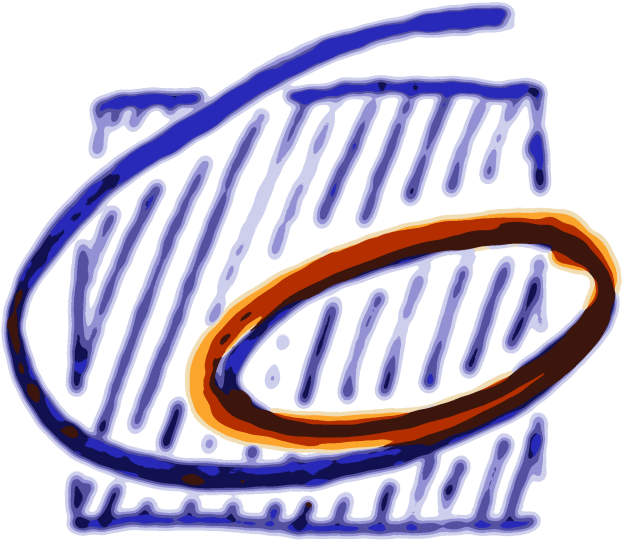
Other analysis features

- Lyapunov exponents
- Parameter scan / sampling



- General sensitivities (first and second order)
- Optimization
- Parameter fitting
- Time scale analysis

The COPASI Team



Blacksburg: Stefan Hoops

Manchester: Pedro Mendes, Joseph Dada

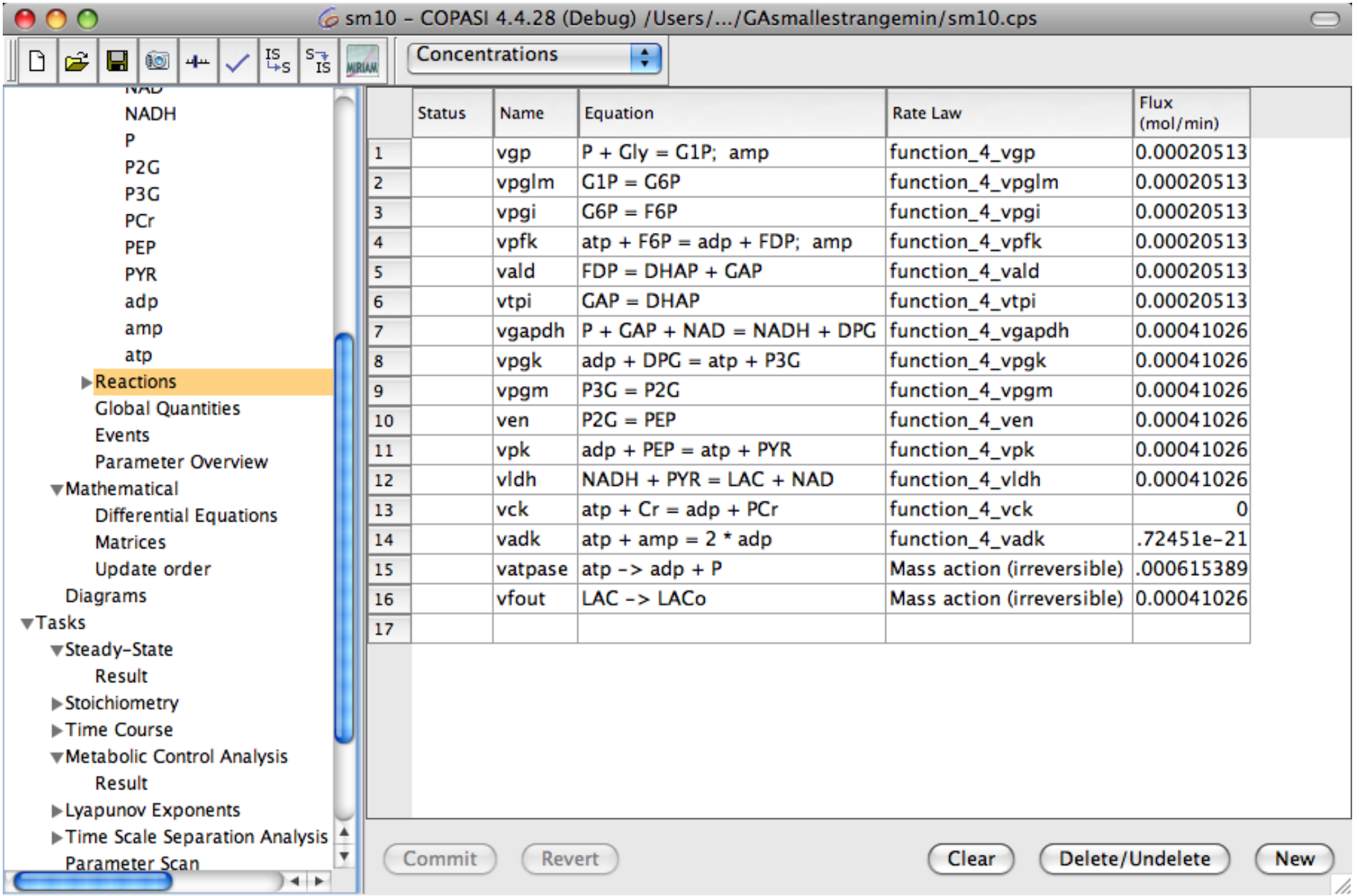
Heidelberg: Ralph Gauges, Ursula Kummer, Natalia Simus, Sven Sahle, Irina Surovtsova

For support: **User forum at www.copasi.org**

We would like to thank the Klaus Tschira Foundation, the BMBF and the NIH for funding.

The model in COPASI

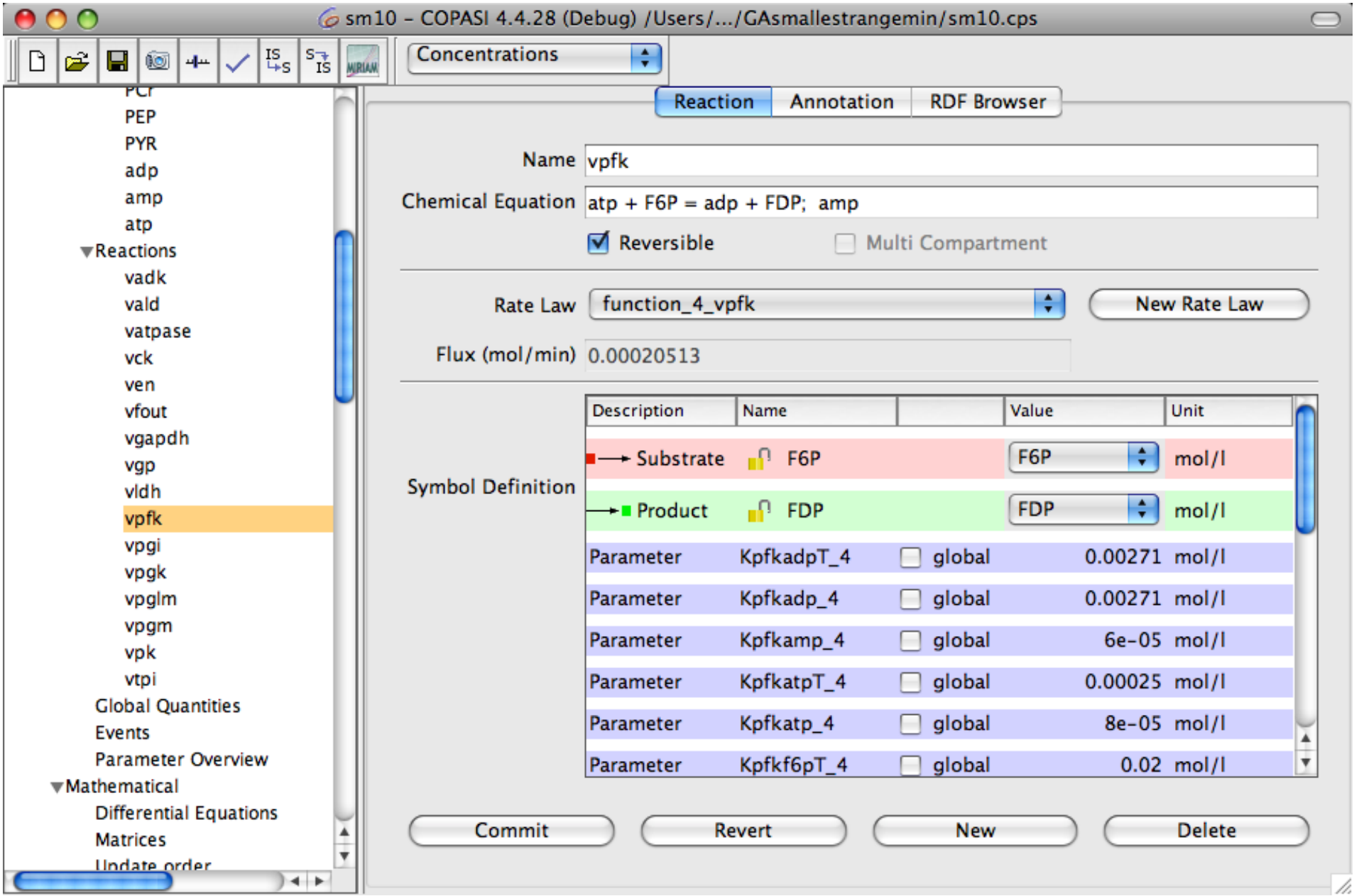
Screenshots



	Status	Name	Equation	Rate Law	Flux (mol/min)
1		vgp	P + Gly = G1P; amp	function_4_vgp	0.00020513
2		vpglm	G1P = G6P	function_4_vpglm	0.00020513
3		vpgi	G6P = F6P	function_4_vpgi	0.00020513
4		vpfk	atp + F6P = adp + FDP; amp	function_4_vpfk	0.00020513
5		vald	FDP = DHAP + GAP	function_4_vald	0.00020513
6		vtpi	GAP = DHAP	function_4_vtpi	0.00020513
7		vgapdh	P + GAP + NAD = NADH + DPG	function_4_vgapdh	0.00041026
8		vpgk	adp + DPG = atp + P3G	function_4_vpgk	0.00041026
9		vpgm	P3G = P2G	function_4_vpgm	0.00041026
10		ven	P2G = PEP	function_4_ven	0.00041026
11		vpk	adp + PEP = atp + PYR	function_4_vpk	0.00041026
12		vldh	NADH + PYR = LAC + NAD	function_4_vldh	0.00041026
13		vck	atp + Cr = adp + PCr	function_4_vck	0
14		vadk	atp + amp = 2 * adp	function_4_vadk	.72451e-21
15		vatpase	atp -> adp + P	Mass action (irreversible)	.000615389
16		vfout	LAC -> LACo	Mass action (irreversible)	0.00041026
17					

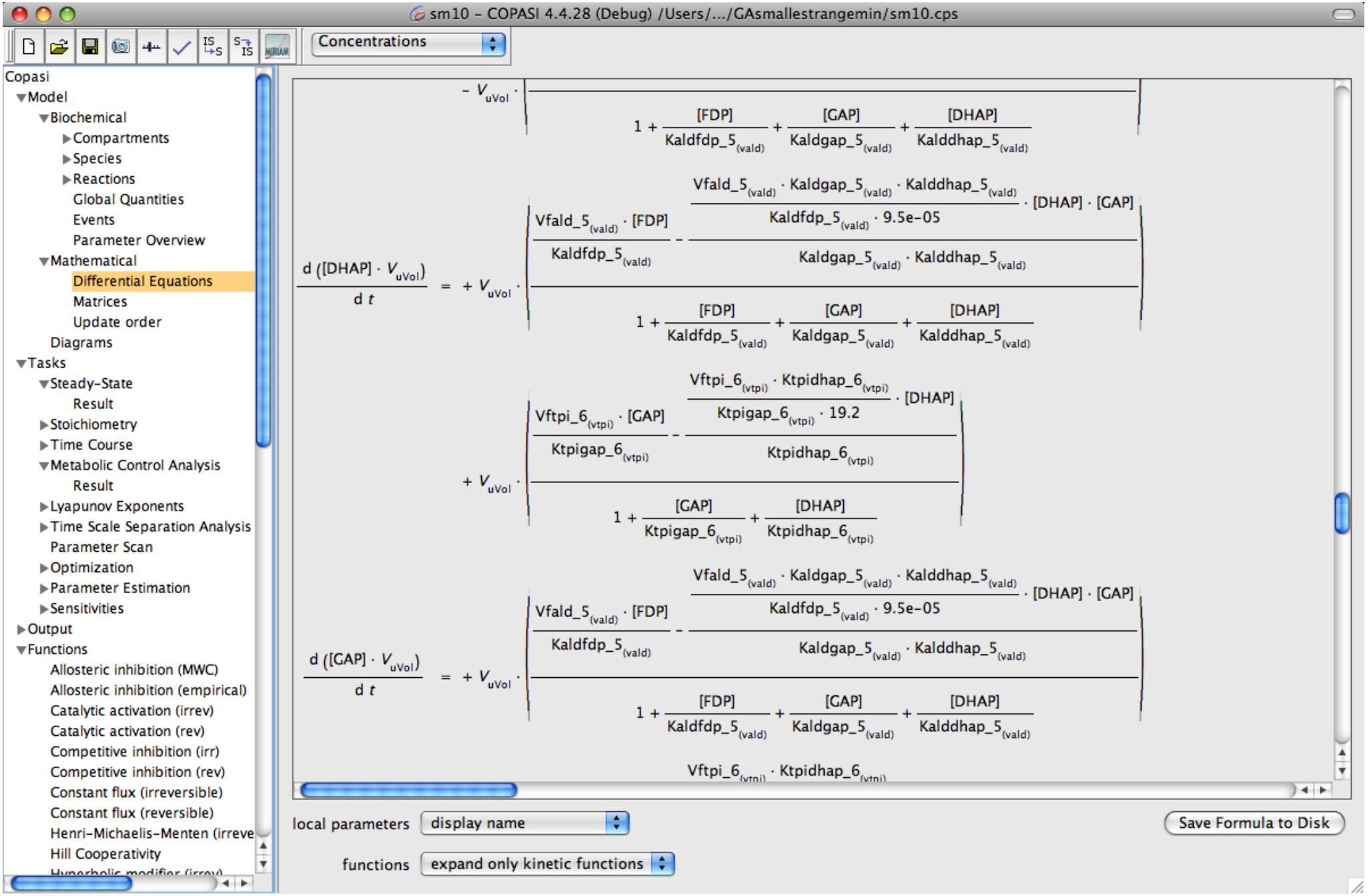
Example (continued)

A reaction in COPASI



ODEs generated from the reaction network

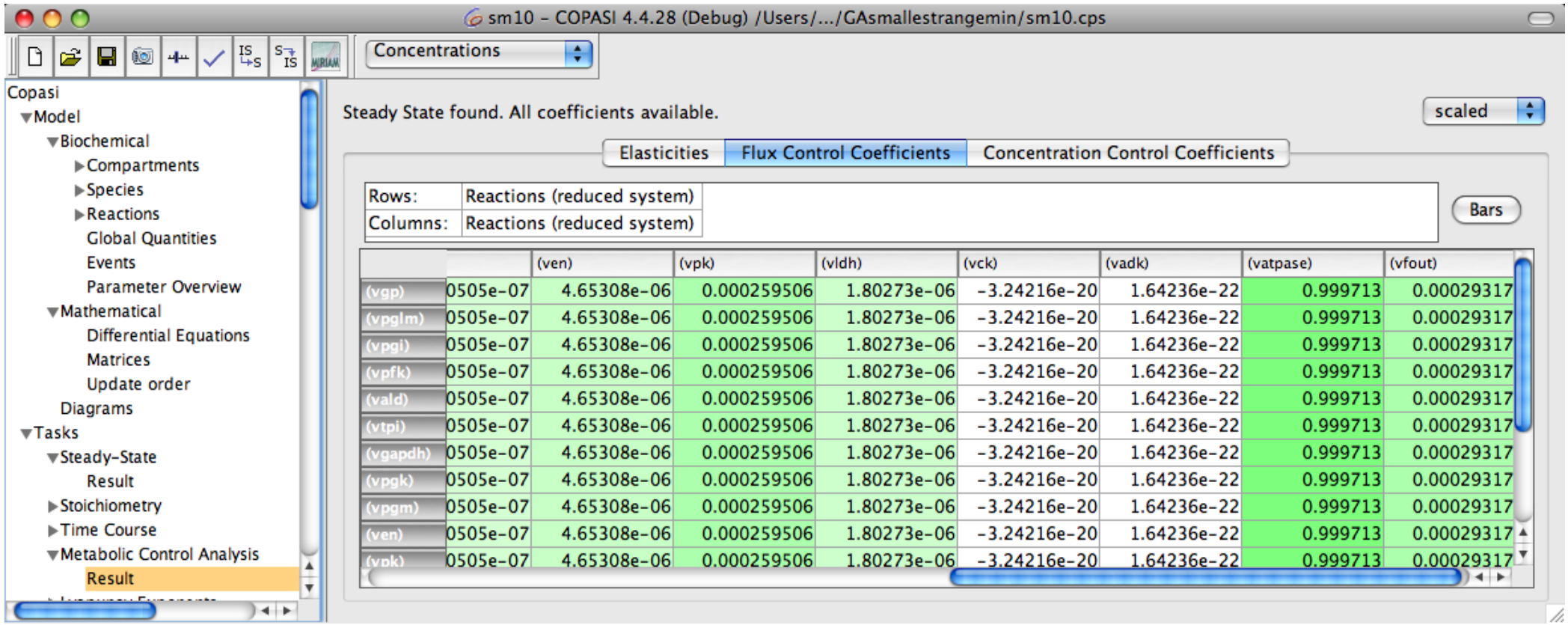
Example
(continued)



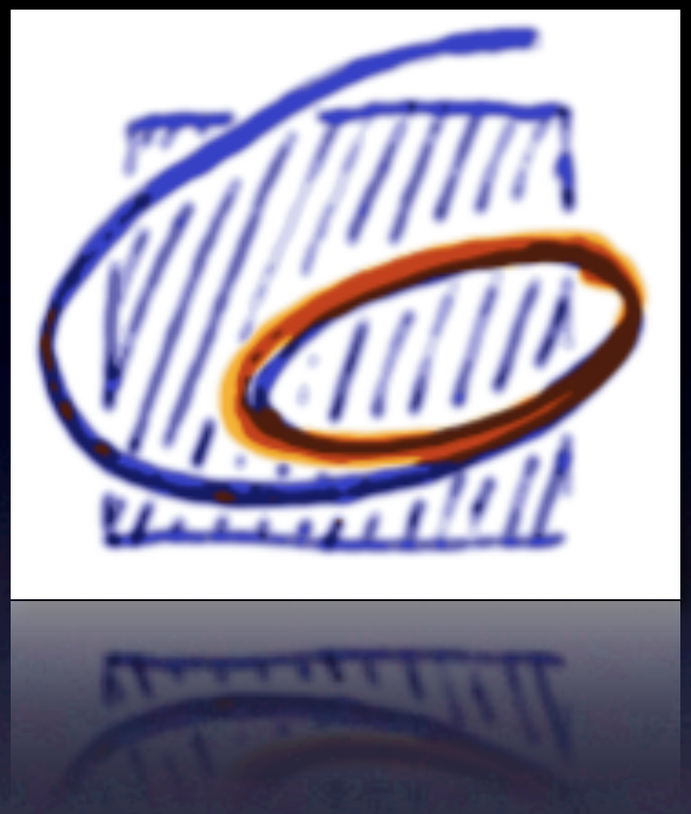
MCA results

Example
(continued)

- For the given parameters the steady state is almost completely controled by the ATPase.



		(ven)	(vpk)	(vldh)	(vck)	(vadk)	(vatpase)	(vfout)
(vgp)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vpglm)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vpgi)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vpfk)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vald)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vtpi)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vgapdh)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vpgk)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vpgm)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(ven)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317
(vpk)	0505e-07	4.65308e-06	0.000259506	1.80273e-06	-3.24216e-20	1.64236e-22	0.999713	0.00029317



COPASI

Integration with other community software

other tools using scripting languages

ModelMage

workflow management systems

SBW

COPASI web services

Condor-COPASI

SYCAMORE

TinkerCell

VCell

CellDesigner

SBSI

multicellular modeling software

CopasiUI
graphical user interface

CopasiSE
command line interface

libCOPASI
C++, python, java
(perl, R, octave)

COPASI

SBW integration

- The GUI version of COPASI has support for the Systems Biology Workbench
- for details about SBW -> Frank Bergmann

Scripting with the COPASI command line interface

- Ideal workflow:
  SED-ML -> COPASI -> SBRML
- current workflow:
  COPASI-ML -> COPASI -> Text file
- example: ModelMage
  (http://sysbio.molgen.mpg.de/modelmage/)

- Condor-COPASI (http://code.google.com/p/condor-copasi/)
  Implemented by Ed Kent in Manchester
    - Web frontend for distributed calculations using COPASI
- COPASI Webservices
  Implemented by Joseph Dada

In both cases we provide the implementation, not the actual service

Both are based on CopasiSE

COPASI language bindings

- COPASI's functionality is available as a library that can be used from a number of programming languages
- C++, python, and java are well supported, perl, R, octave are in progress
- useful documentation is provided
- typically it is released for every stable version of COPASI version
- ask Ralph Gauges for details

Examples

VCell - The Virtual Cell

CellDesigner.org