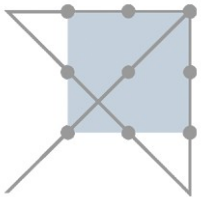


# ***COPASI – A Complex Pathway Simulator***

Surfin' Copasi



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# *What is COPASI?*

- **COPASI** Complex Pathway Simulator

User-friendly and platform-independent tool to access powerful numerical methods for the simulation and analysis of biochemical systems

# *What is COPASI not?*

- only a model editor
- only a simulation library
- only a bunch of analysis methods
- just a plotting tool
- ...
- a database

# *Some technicalities*

- written in **C++**
- uses **Qt** for the GUI and other libraries for the backend (LAPACK, libSBML)
- comes in a **GUI-** and **commandline version**
- runs on **Linux, Windows, Mac OSX** and **Solaris**
- **freely available** under open-source licence for academic users

# *GUI*

- model editing
- plot and report definitions

# *Simulations*

- deterministic: stiff ODE solver **LSODA**
- stochastic: **Gibson and Bruck**
- **hybrid solver**
- easy switch between them

# *Sliders, scans, plots etc.*

- handy **sliders**
- **parameter scans**
- **repeated calculations** including random sampling
- flexible output with **plots** (including histograms) and **reports** (data files)

# *Analysis methods*

- **Conservation relations**
- Elementary flux modes
- **Steady state analysis** (damped Newton method and forward and backward integration) plus stability analysis
- **MCA** (Metabolic Control Analysis)
- **Lyapunov Exponents**



# *Optimization and Parameter Estimation*

- optimization of arbitrary functions
- variety of methods implemented (gradient based methods, random search, evolutionary methods and genetic algorithms)
- support for **steady state** and **time course** experimental data

# ***File format support***

- import and export of **SBML** models (level 1 and 2)
- export of models as **C code**, **Berkeley Madonna**, **XPP**
- **COPASI's native file format** (documentation available)

# Reference

[www.copasi.org](http://www.copasi.org)

(binaries, documentation, tutorials, source code)

S. Hoops, S. Sahle, R. Gauges, C. Lee, J. Pahle, N. Simus, M. Singhal, L. Xu, P. Mendes, U. Kummer (2006)  
“COPASI – a COmplex PATHway Simulator”  
*Bioinformatics* **22**, 3067-74

# Take-home message

- **COPASI** is a tool for the easy access to numerical methods
- It is **platform-independent** and comes with a nice **GUI**
- It provides **deterministic, stochastic and hybrid simulation methods** as well as
- a **variety of methods for the analysis** of your system,
- **optimization, parameter estimation and scans.**
- COPASI supports **SBML** and **outputs other file formats.**
- Freely available for academic use!

# ***COPASI is a joint project***

of

- **Virginia Bioinformatics Inst. in Blacksburg**  
Pedro Mendes (Manchester UK), Stefan Hoops ...
- **EML Research gGmbH in Heidelberg**  
Ursula Kummer (University of Heidelberg),  
Sven Sahle, Ralph Gauges, Jürgen Pahle  
...

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# Questions

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- COPASI can be downloaded from [www.copasi.org](http://www.copasi.org)