

# Simulation Experiment Description Markup Language, an Update



Frank T. Bergmann, PhD  
California Institute of Technology  
University of Heidelberg  
[fbergman@caltech.edu](mailto:fbergman@caltech.edu)



# Simulation Experiment Description Markup Language



- What is it about?
- Where are we?
- Where are we going?

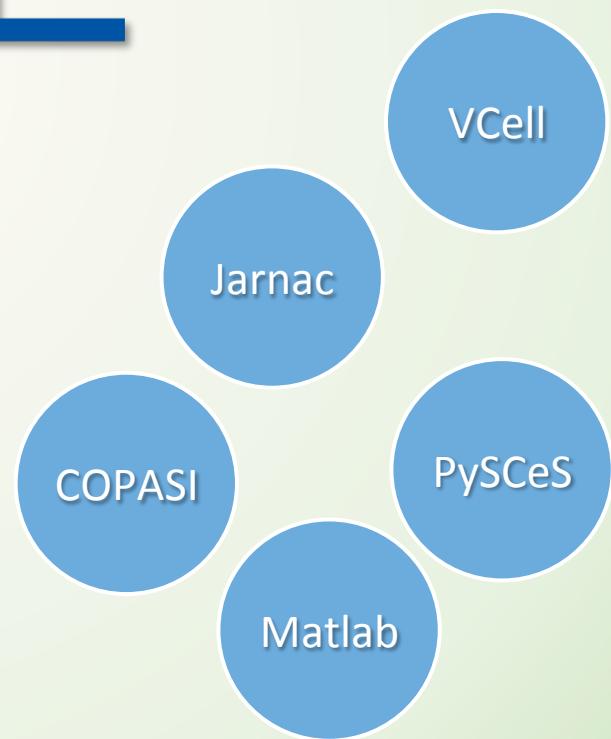
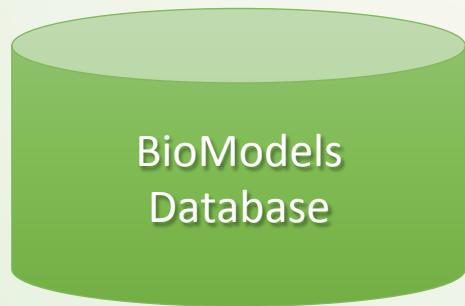
# It all started 2008 ...



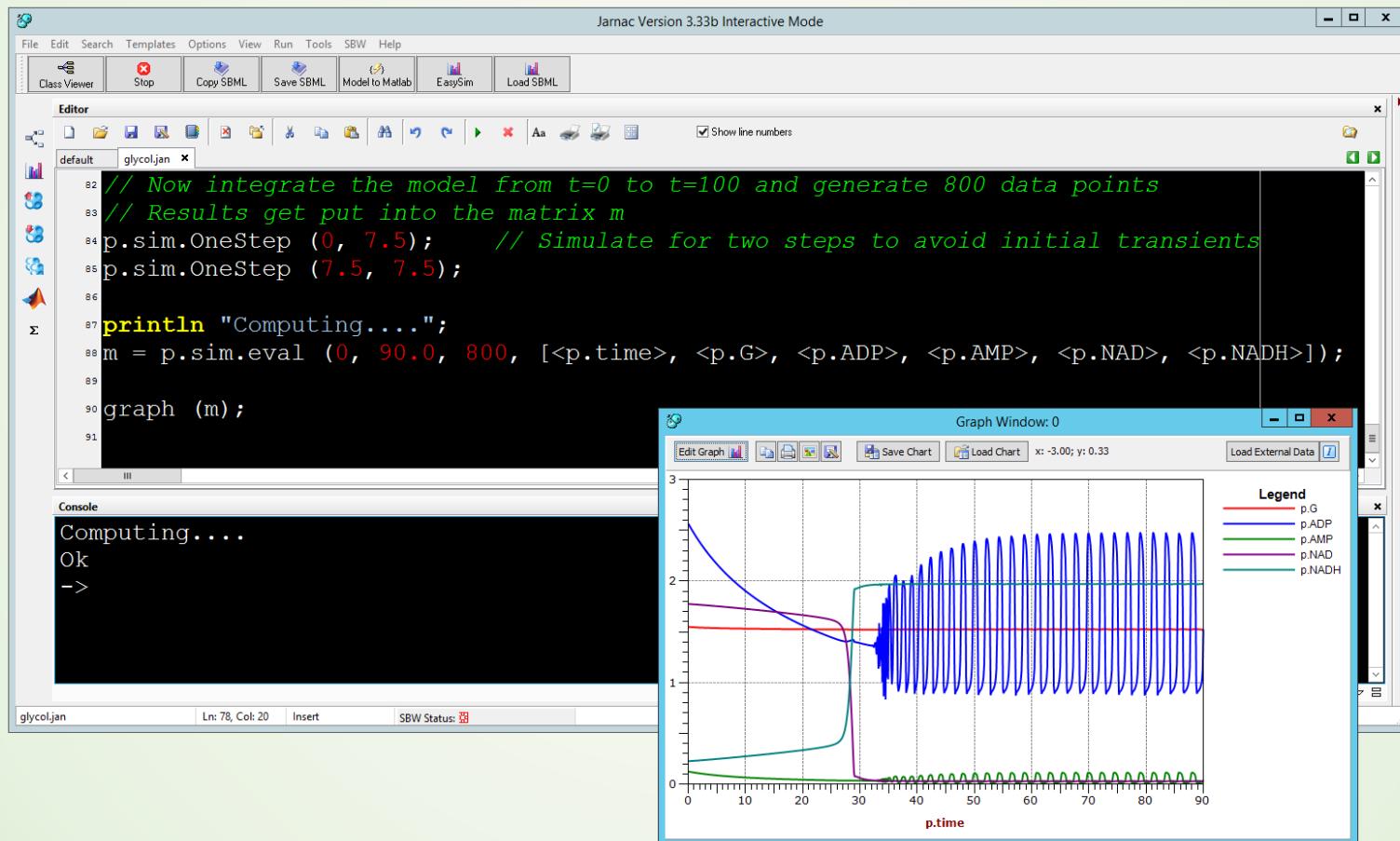
Superhackathon 2008, Okinawa, Picture by Mike Hucka

# Reproducibility

SIM



# Proprietary Solutions



# Proprietary Solutions

```
>>> import scipy  
>>> mod.scan_in = 'x0'  
>>> mod.scan_out = ['J_R1','J_R6','s2_ss','s7_ss']  
>>> scan_range = scipy.linspace(0,100,11)  
>>> mod.Scan1(scan_range)
```

Scanning ...

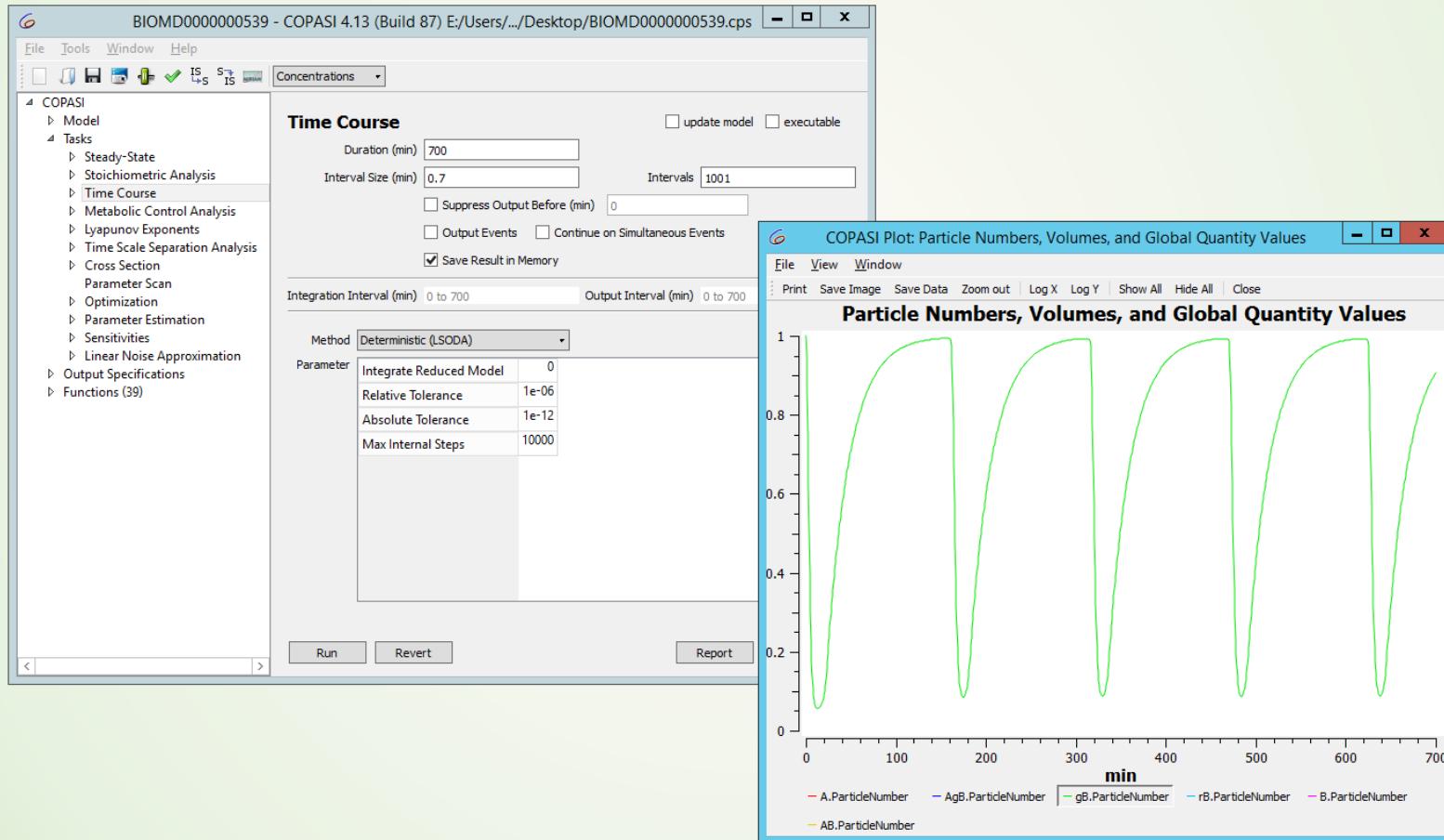
11 (hybrd) The solution converged.

(hybrd) The solution converged ...

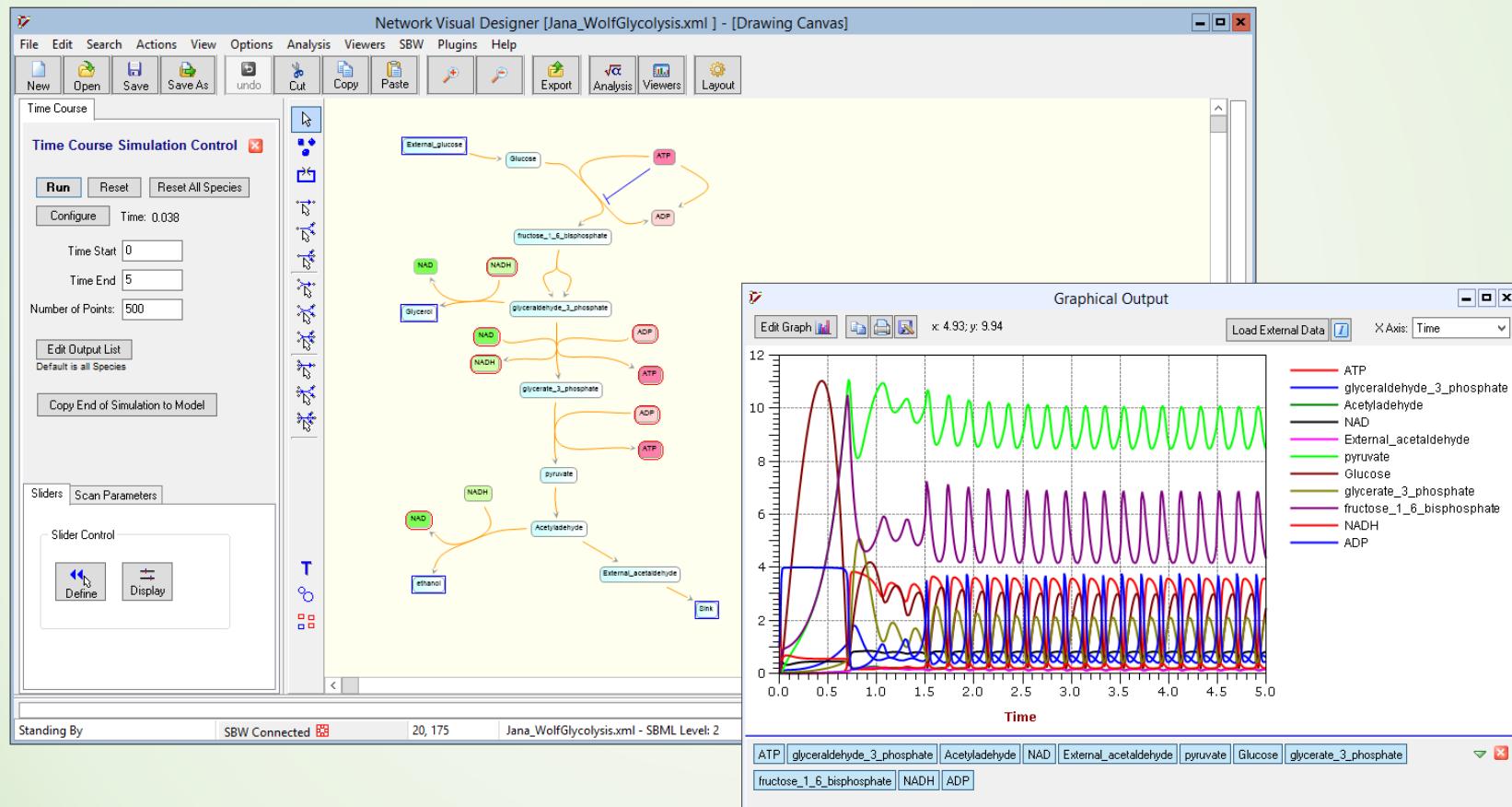
done.

```
>>> mod.Scan1Plot(plot=[], title=None, log=None, format='lines',  
filename=None)
```

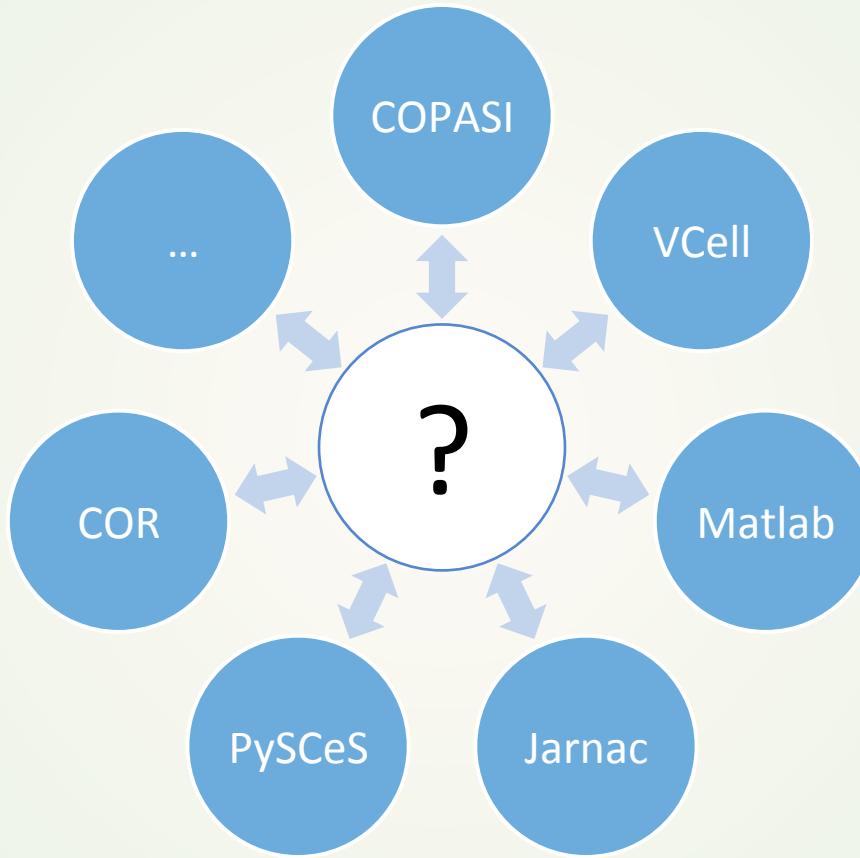
# Proprietary Solutions



# Proprietary Solutions



# Exchange ...

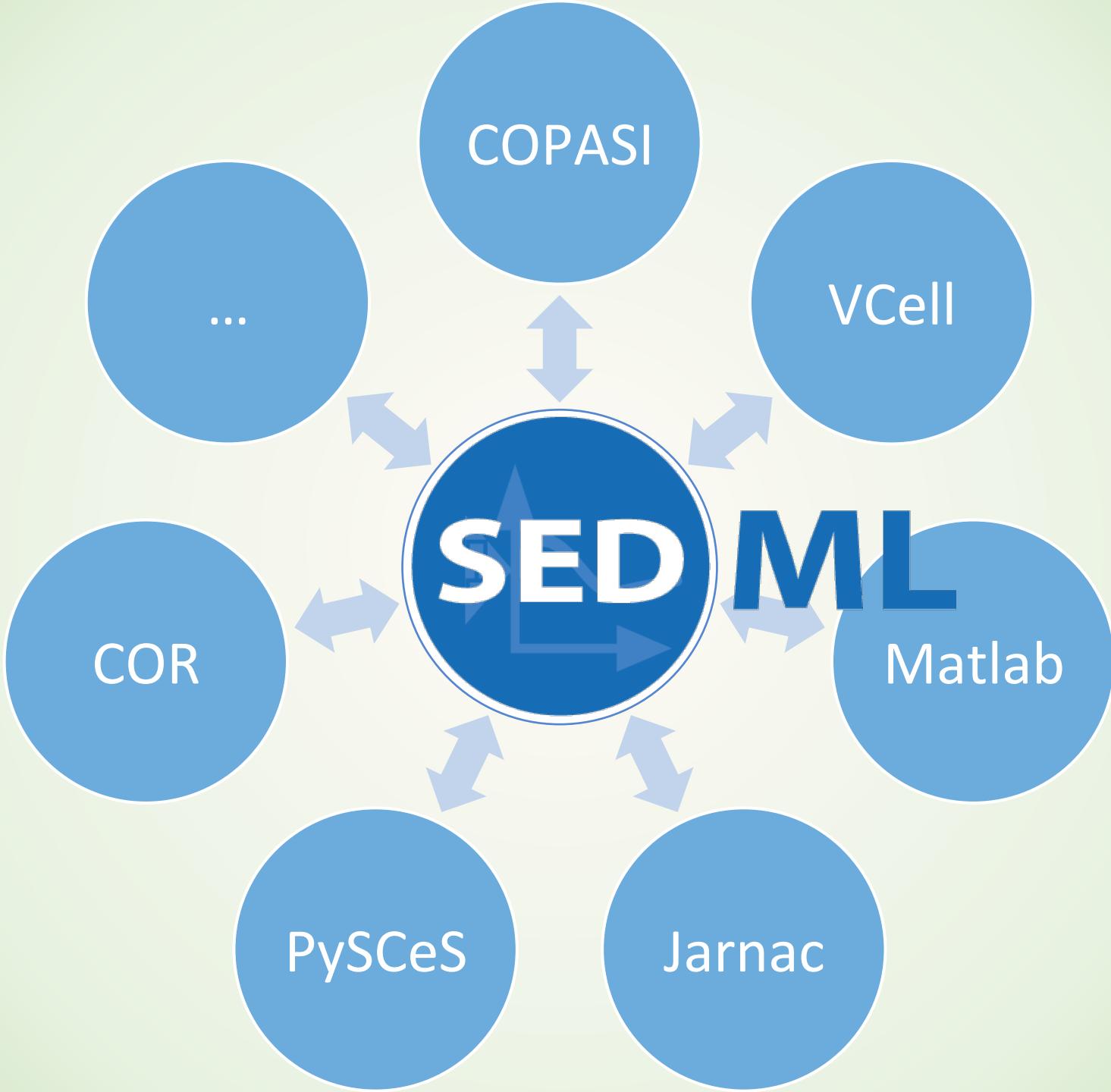


CopasiML  
vCML

NeuroML



SML



# Development Process

- Similar to SBMLs Development Process
- Primary forum online:  
[sed-ml-discuss@lists.sourceforge.net](mailto:sed-ml-discuss@lists.sourceforge.net)
- Editorial Board of 5 Members voted by the community
- Twice yearly meetings
- Regular phone conferences
- Adopt new Specification only if there are two applications implementing it and exchanging descriptions

# KiSAO: Kinetic Simulation Algorithm Ontology



- Defines & relates:
  - Simulation Algorithms
  - Algorithm Parameters

# SED-ML: Repeatable simulation experiments

Model

# SED-ML: Repeatable simulation experiments

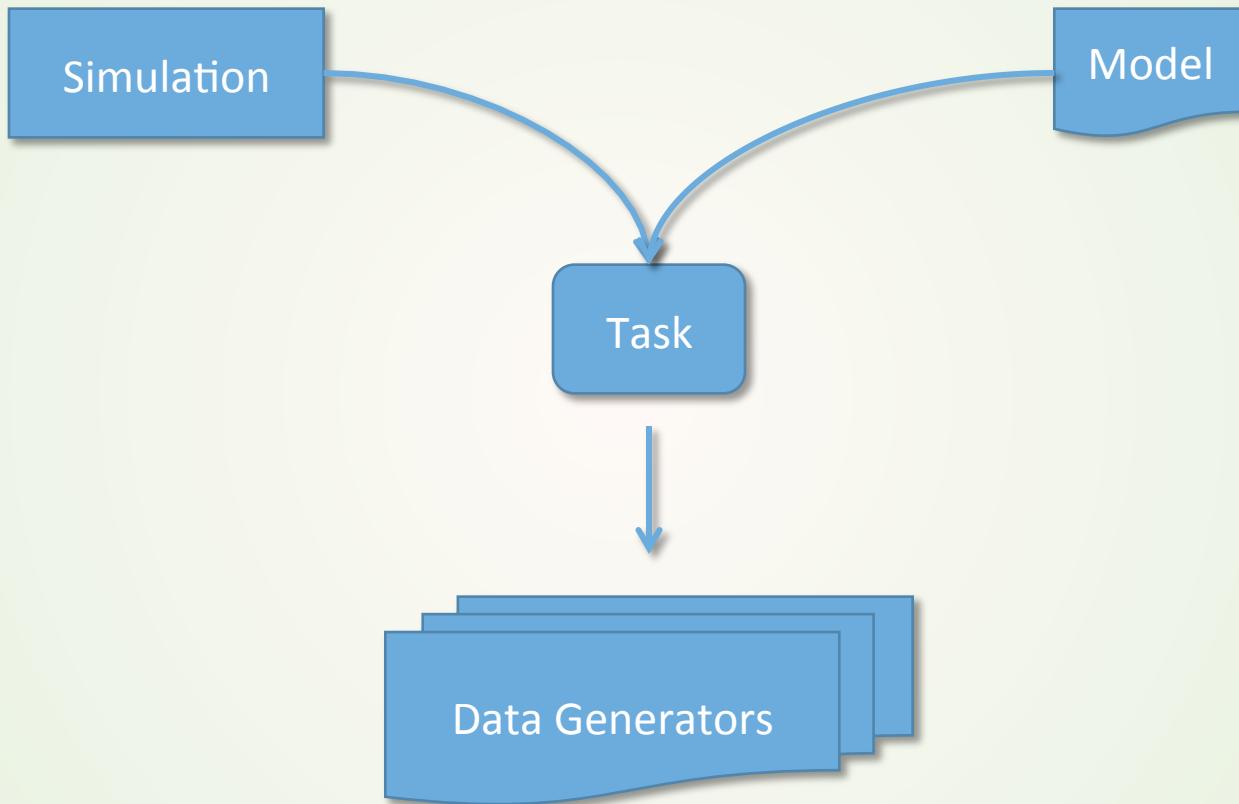
Simulation

Model

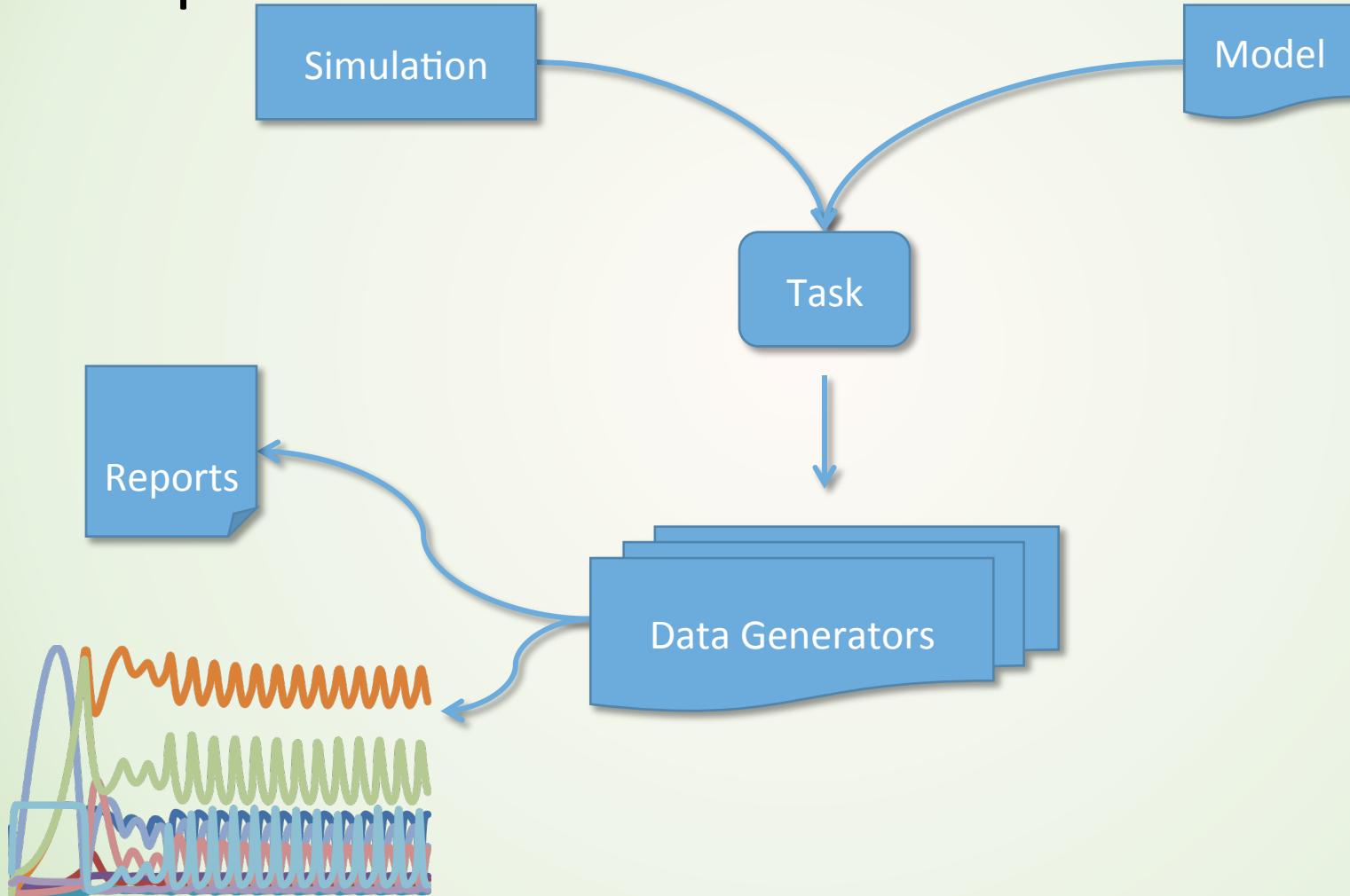
# SED-ML: Repeatable simulation experiments



# SED-ML: Repeatable simulation experiments

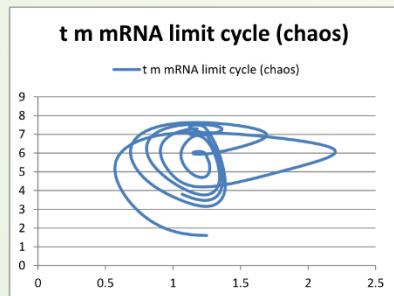
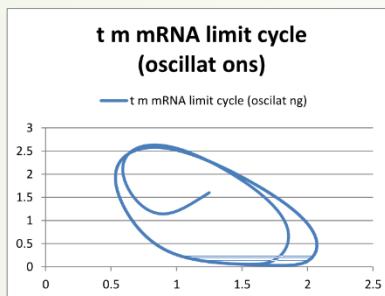
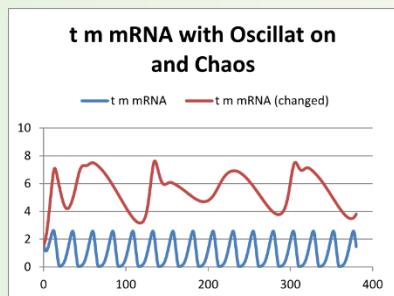


# SED-ML: Repeatable simulation experiments



# Availability

# SED-ML Level 1 Version 1



**Simulation Experiment Description Markup Language (SED-ML) : Level 1 Version 1**

March 25, 2011

**Editors**

Dagmar Waltemath  
Frank T. Bergmann  
Richard Adams  
Nicolas Le Novère  
*University of Rostock, Germany*  
*University of Washington, Seattle, USA*  
*University of Edinburgh, UK*  
*European Bioinformatics Institute, UK*

The latest release of the Level 1 Version 1 specification is available at  
<http://sed-ml.org/>

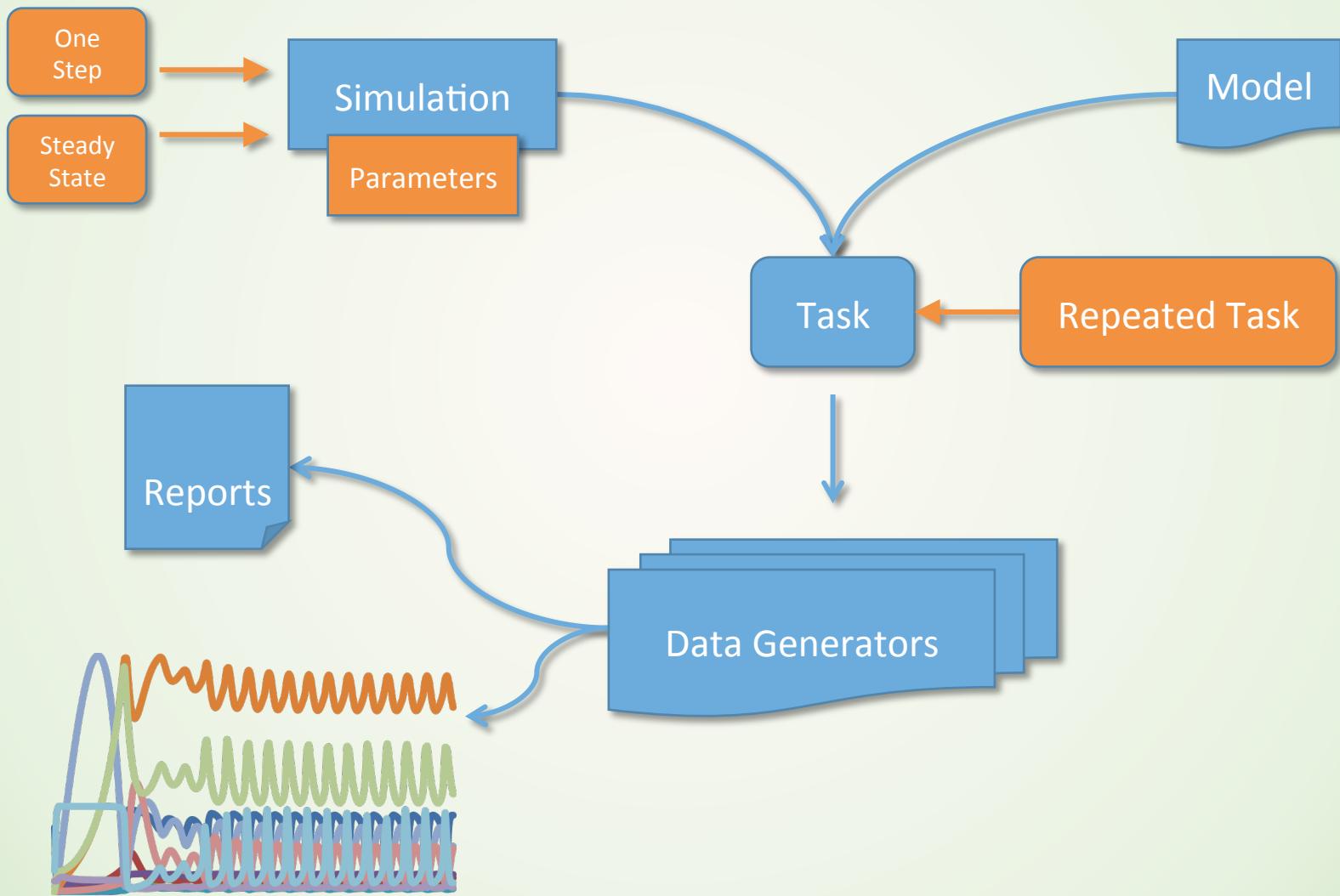
To discuss any aspect of the current SED-ML specification as well as language details, please send your messages to the mailing list  
[sed-ml-discuss@lists.sourceforge.net](mailto:sed-ml-discuss@lists.sourceforge.net).

To get subscribed to the mailing list, please write to the same address  
[sed-ml-discuss@lists.sourceforge.net](mailto:sed-ml-discuss@lists.sourceforge.net).

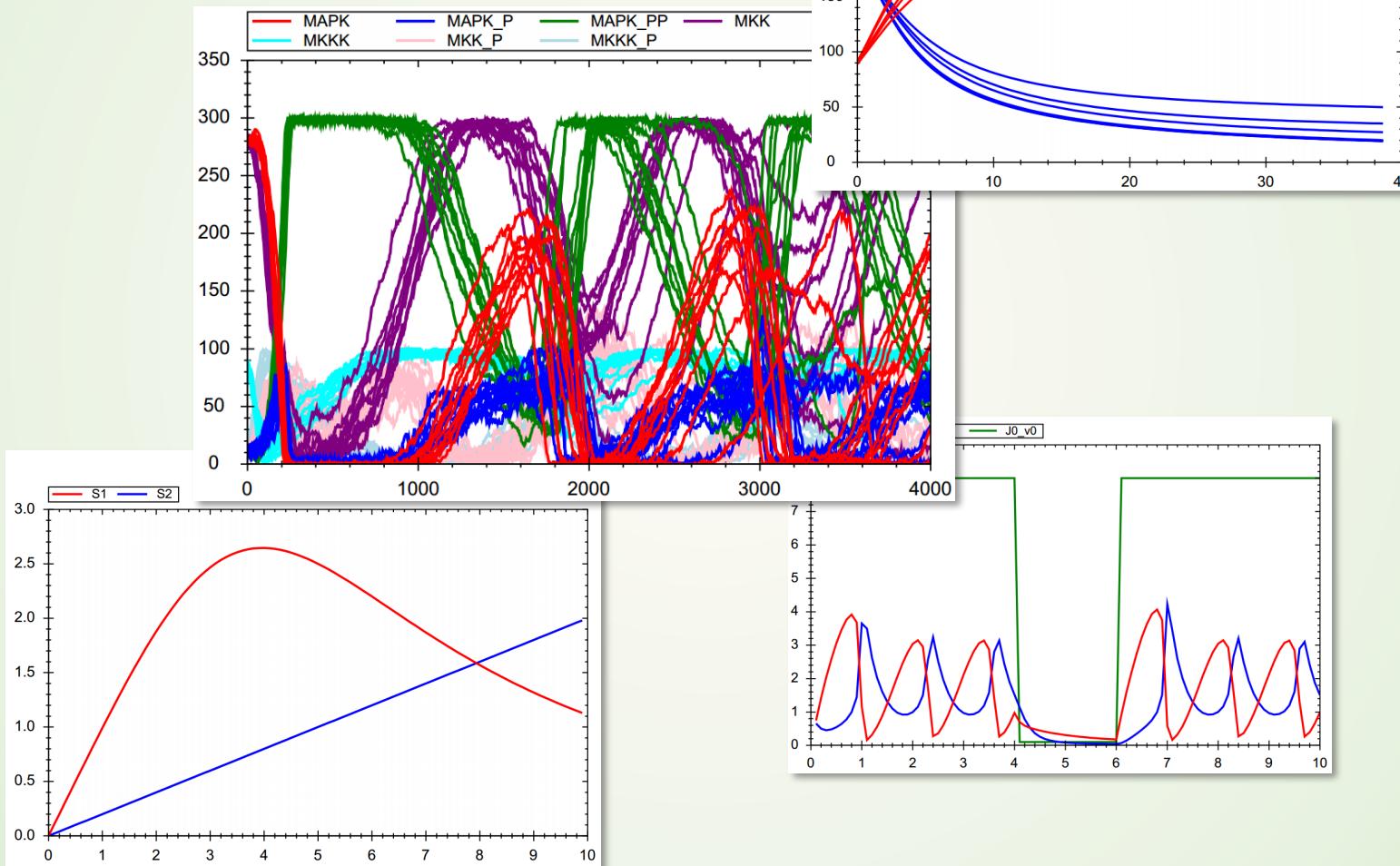
To contact the authors of the SED-ML specification, please write to  
[sed-ml-editors@lists.sourceforge.net](mailto:sed-ml-editors@lists.sourceforge.net)



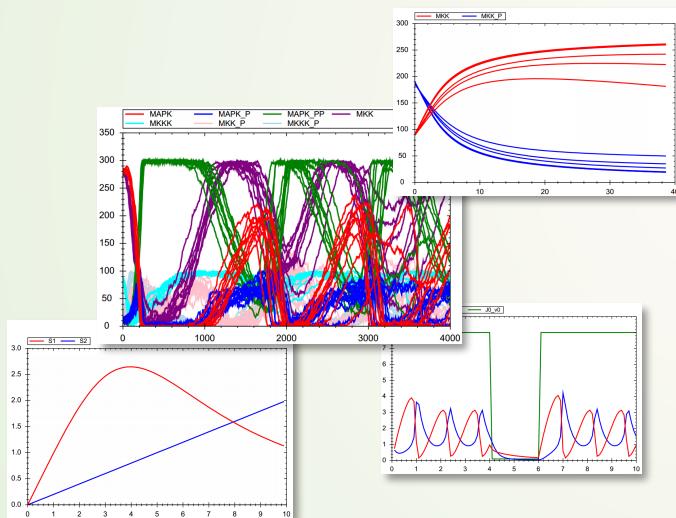
# SED-ML Level 1 Version 2



# SED-ML L1V2



# SED-ML Level 1 Version 2



## Simulation Experiment Description Markup Language (SED-ML) : Level 1 Version 2

December 2, 2013

### Editors

Frank T. Bergmann  
Jonathan Cooper  
Nicolas Le Novère  
David Nickerson  
Dagmar Waltemath  
*University of Washington, Seattle, USA*  
*University of Oxford, UK*  
*European Bioinformatics Institute, UK*  
*Auckland Bioengineering Institute, New Zealand*  
*University of Rostock, Germany*

The latest release of the Level 1 Version 2 specification is available at  
<http://identifiers.org/combine.specifications/sed-ml.level-1.version-2>

To discuss any aspect of the current SED-ML specification as well as language details, please send your messages to the mailing list  
[sed-ml-discuss@lists.sourceforge.net](mailto:sed-ml-discuss@lists.sourceforge.net).

To get subscribed to the mailing list, please write to the same address  
[sed-ml-discuss@lists.sourceforge.net](mailto:sed-ml-discuss@lists.sourceforge.net).

To contact the authors of the SED-ML specification, please write to  
[sed-ml-editors@lists.sourceforge.net](mailto:sed-ml-editors@lists.sourceforge.net)



# Libraries

- libSedML: .NET; BSD License  
<http://libsedml.sourceforge.net>
- libSEDML: *C/C++ with bindings for .NET, Java, Perl, Python, R, Ruby*; BSD License,  
<https://github.com/fbergmann/libsedml>
- jlibsedml: *Java*; MIT License  
<http://sourceforge.net/projects/jlibsedml/>
- clibsedml,: *C*; BSD License  
<http://sourceforge.net/projects/clibsedml/>

# Applications

- CellDesigner
- COPASI
- JWS Online
- PySCeS
- SBSI
- SED-ML Script Editor
- SED-ML Web Tools
- Systems Biology Workbench
- VCell

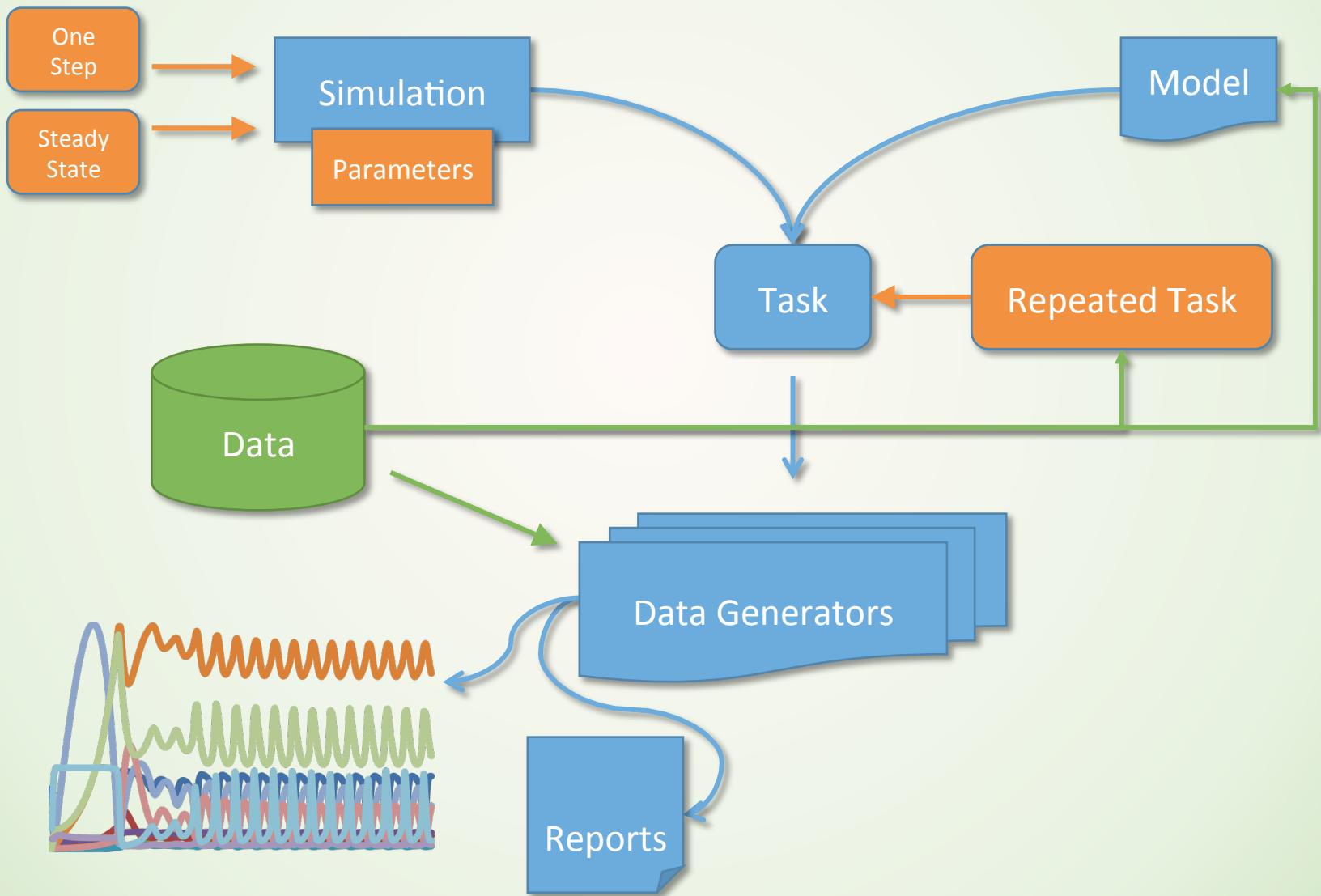
# Extensibility

\annotation/

- Enhanced Output
- Computations involving inaccessible symbols:
  - CC
  - Stoichiometry Matrix
  - Jacobian
  - Eigenvalues ...
- Bifurcation Analysis

# Outlook

# SED-ML Level 1 Version 3



# SED-ML Level 1 Version 3

- Numerical Markup Language:  
<https://code.google.com/p/numl/>
- 1 Prototype implementation available
- Parameter Estimation in discussion

**Simulation Experiment Description Markup  
Language (SED-ML) :  
Level 1 Version 3**

August 17, 2014

**Disclaimer:** This is a working draft of the Simulation Experiment Description Markup Language (SED-ML) Level 1 Version 3 specification. It is not a normative document.

**Editors**

Frank T. Bergmann	<i>University of Heidelberg, Heidelberg, Germany</i>
Jonathan Cooper	<i>University of Oxford, UK</i>
Sven Saale	<i>University of Heidelberg, Heidelberg, Germany</i>
Ion Moraru	<i>University of Connecticut Health Center, US</i>
Dagmar Waltemath	<i>University of Rostock, Germany</i>

The latest release of the Level 1 Version 3 specification is available at  
<http://identifiers.org/combine.specifications/sed-ml.level-1.version-3>

To discuss any aspect of the current SED-ML specification as well as language details, please send your messages to the mailing list  
[sed-ml-discuss@lists.sourceforge.net](mailto:sed-ml-discuss@lists.sourceforge.net).

To get subscribed to the mailing list, please write to the same address  
[sed-ml-discuss@lists.sourceforge.net](mailto:sed-ml-discuss@lists.sourceforge.net).

To contact the authors of the SED-ML specification, please write to  
[sed-ml-editors@lists.sourceforge.net](mailto:sed-ml-editors@lists.sourceforge.net)



# @COMBINE

## Breakouts:

- Wednesday 4pm,
- Thursday 4pm,
- Friday 4pm



Frank Bergmann



Sven Sahle



Ion Moraru

# Acknowledgements

- SED-ML Editors: Frank T. Bergmann, Dagmar Waltemath, Jonathan Cooper, Sven Sahle, Ion Moraru, David Nickerson, Nicolas Le Novère, Andrew Miller, Richard Adams
- BioModels Support Team
- SED-ML Community
- Ursula Kummer, Michael Hucka, Herbert Sauro

